COLLISIONS OF LIGHT NUCLEI

By

Walter Kohn

EREY, CALIF. 93940

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Walter Kohn

Department of Physics
Harvard University
Cambridge, Massachusetts.

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W. Kohn

ABSTRACT

The purpose of this thesis is the investigation of mathematical methods for treating collisions of light nuclei.

Our understanding of nuclear forces is derived largely from the study of simple nuclear systems. Bound nuclei consisting of two to four particles have been theoretically treated with considerable accuracy and yielded many valuable results. Another important source of information are nuclear collisions. However, up to the present, only two particle collisions have been theoretically treated in a systematic and reliable manner.

This thesis is concerned with collisions involving any number of nucleons. The problem is to calculate the scattering properties of nuclei from assumed nuclear interactions. These theoretical results can then be checked against experimental data, thus providing a test for the validity of the interactions which were postulated. As the wave function of a nuclear n - body system extends over 3n dimensions and is highly irregular, on account of the great strength of nuclear forces, one cannot hope to determine it with great exactitude for systems involving more than two particles. For this reason

we have developed variational methods which yield the scattering properties of nuclei with considerable accuracy without requiring an exact knowledge of the wave function.

The wave function is assumed to satisfy a Schroedinger equation in which nuclear forces are described by two-particle, velocity-independent potentials. When the colliding nuclei are far apart, the form of the wave function is known: It consists of a product of functions describing the internal states of the nuclei, and a free particle function, $F(\vec{r})$, of the relative position vector $\vec{r}$ of their centers of gravity. To predict the experimental scattering properties of the nuclei the detailed characteristics of $F(\vec{r})$ must be determined from the assumed interactions.

If one considers collisions in which the nuclei have a definite angular momentum of relative motion, l, the function $F(\vec{r})$ has the asymptotic form

$$F(\vec{r}) \longrightarrow \frac{1}{r}\left(\sin kr + \tan\eta_l \cdot \cos kr\right) S_l,$$

where k is the de Broglie wave number of relative motion, $r = |\vec{r}|$, S_l is the angular function and η_l the phase shift corresponding to the angular momentum l. The phase shift η_l determines the scattering cross section.

Similarly, the function $F(\vec{r})$ corresponding to a plane wave of one nucleus incident on another has the asymptotic form

$$F(\vec{r}) \longrightarrow e^{i\vec{k}_1\cdot\vec{r}} + f(\vec{k}_1, \vec{k})\,\frac{e^{ikr}}{r}.$$

Here $|\vec{k}_1| = |\vec{k}| = k$, $\vec{k}_1$ is in the direction of incidence and $f(\vec{k}_1, \vec{k})$ is the scattering amplitude in the direction of k.

We seek to determine the phase shifts and scattering amplitudes, given the interaction between the nucleons. In collisions of two nucleons the wave equation separates and its solution presents no essential difficulty. But when the colliding nuclei are complex, the Schroedinger equation can no longer be separated. Hence an exact solution is not possible and one must take recourse to approximation methods.

We have followed two lines of attack, both of which have been successful in bound state problems: The Rayleigh-Ritz variational method of undetermined coefficients and the variation-iteration method.

Rayleigh-Ritz Method.

The principle of one of the procedures adopted may be illustrated by the one dimensional Schroedinger equation,

$$\left\{ \frac{d^2}{dx^2} + k^2 - V(x) \right\} u(x) = 0$$

which is to be solved subject to the boundary condition that $u(0) = 0$. The interaction potential $V(x)$ may be supposed to vanish for $x \geq a$, so that

$$u(x) = \sin kx + \tan\eta \cdot \cos kx \,, \qquad x \geq a$$

We now form the expression

$$I = \int_0^\infty u(x) \left\{ \frac{d^2}{dx^2} + k^2 - V(x) \right\} u(x)\, dx$$

and consider its first variation, restricting our trial functions, u_*, by the conditions $u_*(0) = 0$ and

$$u_*(x) \longrightarrow \sin kx + \tan\eta_* \cos kx, \quad \text{as } x \to \infty$$

After an integration by parts, we find

$$\delta I = -k\, \delta(\tan\eta) \quad \text{or:} \quad \delta(I + k \cdot \tan\eta) = 0$$

Since for the correct solution u, $I = 0$, it follows that $\tan\eta$ determined from the equation

$$k \tan\eta = I + k\tan\eta_*$$

is stationary, relative to any admissible variation of u.

When this equation has been re-written in a homogeneous form, one can use a trial function of the type

$$u_* = c_1 u_1 + c_2 u_2 + \cdots c_n u_n$$

on the right hand side and determine the c's from the stationary property of $\tan\eta$. As in the case of bound state problems this leads to a determinantal compatibility equation. In contrast to secular equations this is a <u>linear</u> equation for the determination of $\tan\eta$, regardless of the number of parameters.

This and similar methods are applied to the following cases:

A. Two Particle Collisions.

1. Phase Shifts. Stationary expressions are developed for the phase shifts in the case of central forces and for the proper phase shifts of the scattering matrix in the case of tensor forces. Some numerical calculations show that an accuracy of a fraction of one per cent is attainable without undue labour.

2. Scattering Amplitudes. The variational method developed permits an application of the Rayleigh-Ritz method; it also leads naturally to the Born approximations and Schwinger's variation-iteration formulation (J.S. Schwinger, unpublished lectures).

3. Level Width. A stationary expression for the width of a resonance level is derived.

B. Collisions of Composite Nuclei.

1. Neutron Deuteron Scattering. This case is treated in some detail, as a typical example of composite collisions. A preliminary calculation is carried out for the scattering cross section at zero energy and reasonable agreement (within about ten per cent) is obtained with the experimental value of 3.2 barns.

2. General Composite Collisions. A few features of the Rayleigh-Ritz method in rather general collisions, which may involve excitation or transmutation, are discussed. Variational principles for the elements of the scattering matrix are derived.

Variation Iteration Method.

Instead of employing trial functions with undetermined coefficients in the stationary expressions for the phase shifts and scattering amplitudes one can also use iterated functions.

Thus in the one dimensional problem the n-th iterate is defined in terms of the (n-1)-st by the equation

$$u_n = \int_0^\infty G(x,x')\, V(x')\, u$$

where

$$G(x,x') = \frac{1}{k} \sin k x_< \cdot \cos k x_> + \frac{\cot \eta}{k} \cdot \sin k x \cdot \sin k x'.$$

Professor Schwinger (J. S. Schwinger, unpublished lectures) has applied this method very successfully in collisions of two particles. Since the iteration improves the wave function very rapidly this method converges extremely well. Schwinger's method is generalized from two particle collisions to composite collisions. The persistence of the internal interactions in the asymptotic part of the configuration space causes considerable difficulty in the construction of a suitable Green's function. Of several methods which are investigated only one (involving a Green's function in three dimensions), is found at all feasible. However even this procedure is so complicated, that unless a more suitable version of the variation-iteration method can be found, the Rayleigh-Ritz method appears to be more useful for the treatment of composite nuclear collisions.

J. Schwinger
W. H. Furry
H. Goldstein

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INTRODUCTION.

A great deal of information about the nature of nuclear forces has been derived from a comparison between experimental and theoretical studies of simple nuclear systems. Among the most important data so compared are the binding energy and the magnetic dipole and quadrupole moments of the deuteron[1-3]; the binding energies of H^3, He^3 and He^4[4-6]; and the scattering cross sections of neutrons and protons by protons[7,8].

However, while the binding energies of nuclear 3- and 4-body systems have been theoretically computed and have led to some very important conclusions about nuclear forces (e.g. the forces operative between neutrons[9]), no very satisfactory scheme for mathematically treating collisions which involve more than two elementary particles has so far been given. In what follows some promising methods to solve such problems will be investigated and preliminary results presented.

Theoretical calculations of collisions of light nuclei are worthy of interest for the following reasons:

(1) They may confirm or weaken our confidence in existing nuclear theories; in particular, they may throw light on the

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1. H. A. Bethe and R. F. Bacher, Rev. Mos. Phys. 8, 82 (1936).
2. J. M. B. Kellogg, I. I. Rabi, N. F. Ramsey and J. R. Zacharias, Phys. Rev. 57, 677 (1940).
3. W. Rarita and J. Schwinger, Phys. Rev. 59, 436 (1941).
4. W. Rarita and R. D. Present, Phys. Rev. 51, 788 (1937).
5. H. Margenau and D. T. Warren, Phys. Rev. 52, 790 (1937).
6. E. Gerjuoy and J. Schwinger, Phys. Rev. 61, 138 (1942).
7. L. E. Hoisington, S. S. Share, G. Breit, Phys. Rev. 56, 884 (1939).
8. D. Bohm and C. Richman, Phys. Rev. 71, 567 (1947).
9. R. D. Present, Phys. Rev. 50, 635 (1936).

question whether nuclear forces are, partly, many particle forces.

(2) They may help to decide between certain ambiguities (such as the exact space and spin dependence of nuclear forces), which the data at present available do not settle.

From the very fact that more than two intimately interacting particles are involved it is clear that collisions of composite nuclei present a very complicated theoretical problem. While it is encouraging that the corresponding bound state problems have been solved with a reasonable amount of effort to within a few per cent, it may not be out of place to mention the additional complications of the scattering problems. The asymptotic form of the wave function, instead of having to vanish at infinity, must correctly describe the colliding particles. Above certain energy threshholds it must exhibit the possibility that part of the kinetic energy of collision may be used to raise one or both of the colliding particles to an excited state; or that an exchange of nucleons may take place, so that the resulting nuclei differ from the colliding ones; (e.g. $D^2+D^2 \rightarrow He^3+n^1$); or, finally, that a triple or multiple disintegration may take place (e.g. $Li^7+D^2 \rightarrow$ (intermediate stages) $\rightarrow 2He^4+n^1$). Interactions with the radiation- and electron-neutrino fields will not be considered in this paper. We shall also exclude from our discussion processes in which multiple disintegrations are energetically possible since in that case the asymptotic form of the wave function is very complicated and it was considered

advisable to concentrate first on a solution of the simpler problems.

Experimental Data.

In the last twenty-five years a great many experimental investigations of collisions of light nuclei have been carried out. Many of those performed before 1937 are discussed in Bethe's and Livingston's review articles on "Nuclear Dymanics"[10,11]. A few other typical references are given below[12-14]. Scattering experiments with neutrons as of 1947 have been compiled by H. H. Goldsmith et al.[15]. Quite recently, collisions at very high energies have been investigated by means of the Berkeley cyclotron[16].

It is our general aim to make possible a theoretical interpretation of these experiments. However, this paper is devoted mainly to the development of theoretical methods and only very few numerical calculations have so far been carried out. Hence we shall not be concerned here with a detailed analysis of the experimental data.

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10. H. A. Bethe, Rev. Mos. Phys. 9, 69 (1937).
11. M. S. Livingston and H. A. Bethe, Rev. Mod. Phys. 9, 245 (1937).
12. R. Scherr, J. M. Blair, H. R. Kratz, C. L. Blailey and R. F. Taschek (p-d scattering), Phys. Rev. 72, 662 (1947).
13. R. G. Nuckolls et al.(n-d scattering), Phys. Rev. 70, 805 (1946).
14. N. P. Heydenburg and N. F. Ramsey, Phys. Rev. 60,42 (1941).
15. H. H. Goldsmith, H. W. Ibsen, B. T. Feld, Rev. Mod. Phys. 19, 259 (1947).
16. J. Hadley et al., Bull. A. P. S. 23, 15 (1948).

Previous Theoretical Work.

Theoretical work on more complicated scattering problems has been mostly of a qualitative and phenomenological nature. It has been largely based on the resonance formula of Breit and Wigner[17] which exhibits the scattering process as the temporary formation of a compound nucleus with subsequent emission of the incident or some other particle. In terms of this theory it has been possible to understand the general features of nuclear scattering, but no detailed information about nuclear forces can be derived from it.

Wheeler[18] and Heisenberg[19] have analyzed the general framework of collision processes without going into any detail of the interaction. Their theory serves two purposes: It elucidates the general features of scattering phenomena, regardless of the nature of the interaction, and it represents the first stage of any detailed calculation of composite collisions, based on some specific nuclear theory.

Furthermore, as an approximation to the correct wave function, Wheeler[18] has used functions of so-called group structure, which have been employed in all succeeding calculations. To determine the best possible functions of this sort, he made use of a variational principle. The contents of sections I.6. and I.7. are an extension of this method.

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17. G. Breit and E. Wigner, Phys. Rev. 49, 519 (1936).
18. J. A. Wheeler, Phys. Rev. 52, 1107 (1937).
19. W. Heisenberg, Zs. f. Phys. 120, 513 (1942).

More directly related to the present paper are the works of Schiff[20], Ochiai[21], Flügge[22], Motz and Schwinger[23], Buckingham and Massey[24,25], and Höcker[26] who have calculated scattering cross sections in n-d and p-d collisions from approximate solutions of the Schroedinger equation.

These calculations are all based on a wave function with group structure, that is a function of the form

$$(0.1)\quad \Psi = \sum \psi_i \psi_j F_{ij}$$

where ψ_i , ψ_j describe two collidors i and j when outside their range of interaction, and F_{ij} describes their relative motion. The sum is taken over all pairs of nuclei whose formation is compatible with the given energy and over all permutations of identical particles, with the signs adjusted in accordance with the exclusion principle. The functions F_{ij} are then chosen so that Ψ satisfies the Schroedinger equation as well as possible. A function of this type has the correct symmetry properties and asymptotic behaviour; but in view of the strength of nuclear forces one cannot expect it to approximate too well the correct wave function in that region of the configuration space where the collidors interact, and it is just this region which determines the scattering cross section.

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20. L. I. Schiff, Phys. Rev. 52, 149 (1937).
21. K. Ochiai, Phys. Rev. 52, 1221 (1937).
22. S. Flügge, Zs. f. Phys. 108, 545 (1938).
23. L. Motz and J. Schwinger, Phys. Rev. 58, 26 (1940).
24. R. A. Buckingham and H. S. W. Massey, P. R. S., 123, 179 (1941).
25. R. A. Buckingham and H. S. W. Massey, Phys. Rev. 73,260 (1948).
26. K. H. Höcker, Phys. Zs., 43, 226 (1942).

Of the calculation mentioned above, those of Buckingham and Massey [14,25] are the most extensive. Their method is in essence the following:

The centre of gravity motion of the two neutrons and proton, participating in an n-d collision, is separated out and there remains the following equation for the wave function in the relative coordinates:

$$(0.2)\quad \{T + V_{12} + V_{23} + V_{31}\}\,\Psi = \{E_n + E_d\}\,\Psi .$$

Here T is the kinetic energy operator for the relative motion of the three particles; V_{ij} is the interaction potential between particles i and j, supposed independent of the position of the third particle; E_n is the energy of relative motion of the colliding neutron with respect to the deuteron in the system in which the centre of gravity of all three particles is at rest; and E_d is the binding energy of the deuteron.

Let us introduce relative coordinates to which we shall have frequent reference in the following pages. If R_1, R_2 and R_3 are the absolute position vectors of the two neutrons and the proton, then ρ_1, ρ_2, ρ_3 are defined by

$$(0.3)\quad \begin{aligned} \rho_1 &= R_2 - R_3 \\ \rho_2 &= R_1 - R_3 \\ \rho_3 &= R_1 - R_2 \end{aligned}$$

and similarly r_1, r_2, r_3 are defined by

$$r_1 = R_1 - \frac{R_2+R_3}{2}$$

(0.4) $$r_2 = R_2 - \frac{R_1+R_3}{2}$$

$$r_3 = R_3 - \frac{R_1+R_2}{2}$$

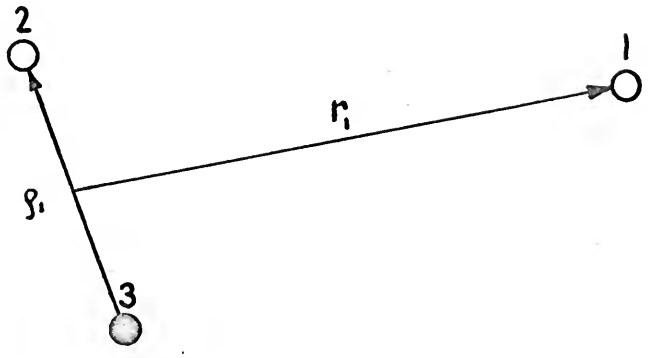

Fig. 1

In terms of these coordinates T has the form

(0.5) $$T = -\frac{\hbar^2}{M}\left(\nabla_{\rho_1}^2 + \frac{3}{2}\nabla_{r_1}^2\right)$$

or the two other forms obtained by replacing 1 by 2 or 3. M is the mass of a nucleon.

The wave function Ψ is a function of the six relative coordinates represented by ρ_1 and r_1 (or any two linear combinations of these) and of the spins of the three particles.

Equation (0.2) is to be solved subject to the condition that when either r_1 or r_2 become large, Ψ describes a deuteron and a free neutron colliding with it. Thus

(0.6) $$\Psi \to \varphi(\rho_1)\left(e^{ik\cdot r_1} + f\frac{e^{ikr_1}}{r_1}\right)\chi_1 \quad \text{as } r_1 \to \infty$$

$$\Psi \to \varphi(\rho_2)\left(e^{ik\cdot r_2} + f\frac{e^{ikr_2}}{r_2}\right)\chi_2 \quad \text{as } r_2 \to \infty.$$

where $\varphi(\rho)$ is the ground-state wave function of the deuteron, $k = |k| = (3\hbar^2 E_4/4M)^{1/2}$, $r_1 = |r_1|$, $r_2 = |r_2|$, f is the scattering amplitude and χ_1 and χ_2 are appropriate spin functions which differ according to whether we consider quartet or doublet scattering.

Although we are not familiar with a rigourous proof that a six-dimensional partial differential equation of elliptic type has a solution which is finite everywhere and satisfies such asymptotic boundary conditions, one intuitively expects this to be the case. However a reasonably rigourous solution is undoubtedly very complicated. Buckingham and Massey, to simplify their problem therefore assume that the exact solution can be <u>everywhere</u> well approximated by a function of the form

$$\Psi = \varphi(\rho_1) F(r_1) \chi_1 + \varphi(\rho_2) F(r_2) \chi_2 . \tag{0.7}$$

This is equivalent to allowing only for the distortion of the free neutron function (since F is as yet undetermined), but disregarding the distortion of the deuteron by the neutron.

To find which function F makes Ψ the best possible solution, they substitute (0.7) into (0.2) and, using the wave equation for the deuteron, they find that F should satisfy, in the case of doublet scattering,

$$\left\{ \frac{3\hbar^2}{4M} \nabla_{r_1}^2 + E_4 - \left(w - \frac{b}{2}\right)(V_{31} + V_{12}) \right\} F(r_1)\, \varphi(\rho_1)$$
$$= \left(w - \frac{b}{2}\right) \left\{ V_{31}\, \varphi(\rho_3) F(r_3) + V_{23}\, \varphi(\rho_2) F(r_2) \right\} . \tag{0.8}$$

Here w, h, m and b represent the strengths of the Wigner, Heisenberg, Majorana and Bartlett forces.

For any fixed value of ρ_1, (0.8) could in principle be solved for $F(r)$ giving $F_{\rho_1}(r)$. But as there is no reason why F should be independent of ρ_1 it is impossible to satisfy (0.8) by a single function $F(r)$. This is just an expression of the fact that a function of the type (0.7) cannot solve the wave equation exactly.

To obtain, as it were, an average solution for F, Buckingham and Massey multiply (0.8) by $\varphi(\rho_1)$ and integrate over the ρ_1-space. This leads to an integro-differential equation for F, of the form

$$(\nabla^2+k^2)\,F(r) = (2w-h)\,U(r)\,F(r) + (2m-b)\int Q(r,r')\,F(r')\,(dr'), \tag{0.9}$$

where U and Q involve the known interaction potentials and the deuteron function. This equation is finally solved by numerical methods.

Previous to Buckingham and Massey, Motz and Schwinger[23] have calculated the scattering of neutrons by deuterons in the zero energy limit. The essential features of their calculation are similar to those of the British workers. Thus, they too consider the deuteron as rigid and are led to an integro-differential equation for the function F. To solve it they replace it by an integral equation according to the scheme:

$$(\nabla^2 + k^2) F(r) = \int K(r, r'') F(r'') (dr'') \longrightarrow$$

(0.10)
$$F(r) = e^{ik \cdot r} + \int \frac{e^{ik|r-r'|}}{4\pi |r-r'|} K(r', r'') F(r'') (dr'') (dr').$$

After carrying out angular integrations analytically the remaining integral equation is solved approximately by replacing it by a set of simultaneous linear equations.

Finally, Höcker[26] has tried to write $F(r)$ as a power series in λ and determine the coefficients to best fit the Schroedinger equation. However his results depend, by a factor of about 1.5-2.0 on the point where the power-series is taken to pass over into the asymptotic form of F.

The other calculations do not contain any essentially different methods.

The different authors using various kinds of (central) interactions obtained widely different results. For the total cross section of n-d scattering at 0-energy they are in units of barns as follows: Schiff[20] : 6.11 ; Ochiai[21] : 3.2 ; Motz and Schwinger[23] : 4.57, 6.91 ; Buckingham and Massey[24] : 3.0, 3.9 (extrapolated) ; Höcker[26] : 1.88, 2.95 . The experimental value is near 3.3[13,27].

Other two- and three-particle systems do not exhibit such a strong dependence on the type of interaction, at low energies. If taken at their face value, then, these results would provide a useful method for distinguishing between various kinds of interaction, all of which are compatible with other

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27. L. J. Rainwater et al., Phys. Rev. 73, 733 (1948).

low energy phenomena.

However, such a procedure would be without firm foundation in view of the unreliability of the group structure function, on which all calculations are based. This emphasises the need for a systematic method of solution, which is not restricted to any particular kind of function.

Summary of the Present Paper.

It is not the primary purpose of this paper to add another approximate calculation to those already published, but rather to investigate the possibility of a systematic procedure for solving the Schroedinger equations corresponding to composite scattering processes. It was natural to look for a variational method, as this has been the chief tool for solving the problems of the bound 3- and 4-particle systems[4-6, 28] and has recently been applied by Schwinger[29] to 2-particle scattering problems.

There are two types of practical variation procedures: One is the Rayleigh-Ritz method[30] of undetermined coefficients; the other the variation iteration method[28,29] employing Green's functions. We have tried both methods in the many particle scattering problem, and we strongly incline to the opinion that the

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28. N. Svartholm, Thesis, Lund, Hakan Ohlssons, Boktryckeri (1945).
29. Unpublished lectures.
30. W. Ritz, J. reine angew. Math. 135 (1909).

Rayleigh-Ritz method is the more useful.

Using this method we have made exploratory calculations on 2- and 3-particle scattering problems, some with the inclusion of tensor forces. On the basis of these we believe that this procedure can indeed be used for a systematic investigation of collisions of light nuclei.

I. THE RAYLEIGH-RITZ METHOD IN COLLISION PROBLEMS.

I.1. General Remarks.

In his original paper on wave mechanics, Schroedinger derived the wave equation from a variational principle analogous to Hamilton's Principle in classical mechanics. The variational formulation of the equations of motion of wave-fields has been very fruitful not only in theoretical developments of field theory[32] but also in approximate solutions of complicated quantum mechanical problems[33].

The method most extensively used in practical problems has been the Rayleigh-Ritz method[30] of linear trial functions. However its application has been limited to systems in bound states, whose wave functions vanish rapidly at infinity.

Recently, Heisenberg[19] has pointed out the correspondence between the phase shift energy relation of a collision problem and the energy spectrum obtained if the participating particles are enclosed in a large box.

Consider, as the simplest example, a particle of mass M under the action of a short range scattering centre. The wave equation for the radial part of the spherically symmetric solution is

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31. E. Schroedinger, Ann. d. Phys. 79, 361 (1926).
32. See, for example, G. Wentzel, "Einführung in die Quantentheorie d. Wellenfelder", Wien, Franz Deuticke (1943).
33. E. Hylleraas, Zs. f. Phys. 54, 347 (1929).

$$(1.1)\quad \left\{ -\frac{\hbar^2}{2M}\frac{d^2}{dr^2} + U(r) \right\} u(r) = E\,u(r),$$

where $U(r)$ is the scattering potential and E the total energy. Asymptotically the solution becomes

$$(1.2)\quad u \longrightarrow \sin\left(\sqrt{\frac{2ME}{\hbar^2}}\, r + \eta(E)\right),$$

where the phase shift $\eta(E)$, corresponding to the energy E of the incident particle must be found by a detailed solution of (1.1).

Now let us ask for the energy levels of the same particle in the same potential field when enclosed in a spherical box of large radius, a, on which the wave function must vanish. Since the differential equation is unchanged, all those solutions of the scattering problem will satisfy the bound state problem for which

$$(1.3)\quad \sin\left(\sqrt{\frac{2ME}{\hbar^2}}\, a + \eta(E)\right) = 0.$$

It is clear that if we have solved the scattering problem and determined the function $\eta(E)$ we can find the energy levels, E_i, of the bound particle by solving (1.3) for E; and conversely if the spectrum, E_i, of the bound particle has been determined the phase shifts $\eta(E_i)$ can be found from (1.3).

These considerations lead us to expect that the Rayleigh-Ritz method, which has been so valuable for

calculations of energy levels of bound systems, will apply, with certain modifications to the calculation of phase shifts and scattering amplitudes.

I.2. Three Related Treatments of One Dimensional Problems. The Collision Determinant. Numerical Illustrations.

In this section we shall illustrate our methods by treating the scattering of a particle by a fixed, short range scattering centre. We shall show that this problem can be attacked in three closely related ways.

Let us first simplify the Schroedinger equation (1.1) by introducing a convenient unit of length, r_0, and writing

$$(2.1)\quad x = \frac{r}{r_0}\,, \quad K^2 = \frac{2ME}{\hbar^2} r_0^2\,, \quad V(x) = \frac{2MU(r_0 x)}{\hbar^2} r_0^2 .$$

It then becomes

$$(2.2)\quad \left[\frac{d^2}{dx^2} + K^2 - V(x)\right] u(x) = 0$$

It will be our problem to solve (1.5) subject to the conditions that

$$(2.3)\quad u(0) = 0\,, \quad u(x) \longrightarrow \sin Kx + \tan\eta \cos Kx \quad \text{as } x \to \infty .$$

In particular we are interested in the phase shift which determines the scattering cross section.

Method 1: The Energy as Proper Value.

We know that (2.2) and (2.3) have a solution for every positive K. However, instead of looking for the phase shift corresponding to a given K, we can reverse the problem and ask for the K corresponding to a given logarithmic derivative, L, of u at some large distance a. This means we look for the proper value κ^2 belonging to the differential equation (2.2) and the boundary conditions

$$(2.4) \qquad u(0) = 0 \,, \quad u'(a) = L\,u(a).$$

This is a proper value problem of a standard type [34] and it is easily verified that κ^2 as calculated from the equation

$$(2.5) \qquad \int_0^a \left\{ -u'^2 + K^2 u^2 - V u^2 \right\} dx + L\,u^2(a) = 0$$

is stationary with respect to all variations of u which satisfy the condition $\delta u(0) = 0$.

The Rayleigh-Ritz method is directly applicable to (2.5). We simply try for u a linear combination of trial functions

$$(2.6) \qquad u = c_1 u_1(x) + c_2 u_2(x) + \cdots \qquad c_n u_n(x)$$

(with all $u_i(0) = 0$) and substitute this expression into (2.5). This leads to an equation of the form

$$(2.7) \qquad Q \equiv \sum_{\substack{i=1 \\ j=1}} \left(A_{ij} + B_{ij} K^2 \right) c_i c_j = 0$$

where A_{ij}, B_{ij} are integrals involving u_i and u_j.

34. R. Courant and D. Hilbert, Methoden d. Math. Physik, vol. II, 508, Berlin, Springer, 1937.

The stationary property of K^2 with respect to variations of the c_i leads to the following system of equations for the determination of these coefficients:

$$\frac{\partial Q}{\partial c_i} = 2 \sum_j \left(A_{ij} + B_{ij} K^2 \right) c_j = 0 \qquad i = 1, 2, \ldots n. \tag{2.8}$$

As in the case of the bound state problem this system is compatible only if K^2 has certain proper values K_ℓ^2 which can be found by the solution of the corresponding secular equation. They are approximations to the correct proper values of (2.2) under the boundary conditions (2.4). Their errors are of the order of the square of the errors of the trial functions.

Now the phase shifts of the exact solutions corresponding to the given L satisfy the equation

$$K \cot \left(Ka + \eta(K) \right) = L . \tag{2.9}$$

If we substitute our approximations K_ℓ in this equation we obtain, to the same (namely the second) order of accuracy, values for $\eta \left(K_\ell \right)$ corresponding to the energies K_ℓ^2 . Then, either by varying the pre-assigned value of L or the "cut-off" distance a, we can obtain η for all other energies.

In this form of the variational method, we have followed very closely the analogy between bound and unbound systems pointed out by Heisenberg. However the quantization of the

energy which entails the necessity for solving a secular equation of the usual kind seems artificial and can indeed be avoided.

Method 2. The Logarithmic Derivative as Extremum.

Since for a given L, K^2 as calculated from (2.5) is stationary, so also must L be stationary when calculated with a given K^2. Using the trial functions (2.6) we are led again to (2.7), but now we take K^2 as fixed and L as adjustable so as to make the ensuing system of equations compatible. Therefore we exhibit L explicitely and write Q in the form

$$Q = \sum_{\substack{i=1 \\ j=1}}^{n} C_{ij}(K^2) c_i c_j + L\{c_1 u_1(a) + c_2 u_2(a) + \cdots c_n u_n(a)\}^2 = 0 \tag{2.10}$$

It is convenient to transform the coefficients c_i to a new set d_i as follows:

$$d_1 = c_1 u_1(a) + c_2 u_2(a) + \cdots c_n u_n(a)$$
$$d_i = c_i \qquad i = 2, 3, \ldots n \tag{2.11}$$

In terms of the d_i, Q has the form

$$Q = \sum_{\substack{i=1 \\ j=1}} D_{ij}(K^2)\, d_i d_j + L d_1^2 = 0 \tag{2.12}$$

The stationary property of L with respect to variations of the d_i now leads to the equations

$$\sum_{j=1}^{n} D_{1j}(K^2)\, d_j + L\, d_1 = 0$$

$$\sum_{j=1}^{n} D_{ij}(K^2)\, d_j = 0 \quad , \qquad i = 2, 3, \ldots n. \tag{2.13}$$

To make the system of equations (2.13) compatible L must satisfy the determinantal equation

$$\Delta \equiv \begin{vmatrix} L + D_{11} & D_{12} & \cdots & D_{1n} \\ D_{21} & D_{22} & \cdots & D_{2n} \\ \vdots & \vdots & & \vdots \\ D_{n1} & D_{n2} & \cdots & D_{nn} \end{vmatrix} = 0. \tag{2.14}$$

Hence L is a quotient of two determinants, each of which is a function of K^2 .

Let us note that Δ is symmetrical and of degree 1 in L, in contra-distinction to the secular determinants in problems of the bound state, whose degree in the unknown energy is as high as the number of trial functions. We shall see later (sections I.5. - I.7.) that the structure of Δ or of the corresponding determinant occurring in method 3 reflects the type of the collision and for this reason call it a collision determinant [35] . Its degree in L is of course

35. It is related to Wheeler's Fredholm determinant, ref. 18, eq.(45).

invariant under the transformation (2.11) which was introduced only for reasons of greater clarity. Indeed one can easily verify that the determinantal equation for L, as deduced directly from (2.10),

$$(2.15) \qquad \left| C_{ij} + L\, u_i(a)\, u_j(a) \right| = 0$$

is also of the first degree in L, since the matrix $\| u_i(a)\, u_j(a) \|$ of the coefficients of L has rank 1.

There remains as an unsatisfactory feature of this treatment the dependence of the phase shift, deduced from K^2 and L, on the cut-off distance a, even when a is well beyond the range of interaction. This question will be discussed in more detail further on in this section. Meanwhile we shall indicate another method which does not have this drawback.

Method 3. The Tangent of the Phase Shift as Extremum.

Let us return to equation (2.2) and (writing ϵ instead of K^2) note that, in the bound state, ϵ calculated from

$$(2.16) \qquad I \equiv \int_0^\infty u \left\{ \frac{d^2}{dx^2} + \epsilon - V(x) \right\} u \; dx = 0$$

is stationary relative to all variations of u with $\delta u(0) = 0$ and $\delta u(\infty) = 0$. For,

$$(2.17) \qquad \delta I = 2 \int_0^\infty \delta u \left\{ \frac{d^2}{dx^2} + \epsilon - V(x) \right\} u \; dx + \left[u \frac{d}{dx} \delta u - \delta u \frac{d}{dx} u \right]_0^\infty$$

and both the integrand and integrated terms vanish.

In a collision, however, the wave function has the form (2.3) at infinity. If we restrict our trial functions to those having the correct asymptotic form, although possibly wrong phase shift, then

$$\delta u \to \delta \tan\eta \cdot \cos kx \,, \quad \text{as } x \to \infty. \tag{2.18}$$

Hence

$$u \frac{d}{dx}\delta u - \delta u \frac{d}{dx} u \Big|_{x=\infty} = k\,\delta \tan\eta, \tag{2.19}$$

so that

$$\delta\left(I + k\tan\eta\right) = 0.^{36} \tag{2.20}$$

Since for the correct wave function $I = 0$, it follows that the equation

$$I + k\tan\eta_* = k\tan\eta, \tag{2.21}$$

where η_* is the trial phase shift, is a stationary expression for $\tan\eta$.

To apply the Rayleigh- Ritz method it is essential to write this variational principle in a homogeneous form. Let us therefore consider wave functions of the asymptotic form

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36. L. Hulthen (Extrait, Dixieme Congres des Mathematiciens Scandinaves, Copenhague, 1946) has used an equivalent equation to find η by further restricting his wave functions to satisfy the condition $I = 0$.

(2.22) $u \longrightarrow A \sin Kx + B \cos Kx$

instead of (2.3). We then find in the same way as above

(2.23) $$I + AB K = A^2 K \tan \eta$$

as a homogeneous variational principle for $\tan \eta$. If we use a trial function of the form

(2.24) $$u = A \sin Kx + c_2 u_2 + \cdots c_n u_n$$

where

(2.25) $$c_2 u_2 + c_3 u_3 + \cdots c_n u_n \longrightarrow B \cos Kx,$$

then since $\tan \eta$ multiplies only A^2, substitution of (2.24) into (2.23) will give a quadratic form of the same structure as (2.12) which in turn will again lead to a linear collision determinant for $\tan \eta$.

The drawback of this formulation is that the trial functions must be of the form (2.24), (2.25). For practical purposes it may therefore be preferable to re-adopt a finite cut-off as follows: Let a be a distance beyond which the interaction is negligible and let us use as trial function

(2.26)
$$u = u^{(i)} = c_1 u_1 + c_2 u_2 + \cdots c_n u_n, \quad x \leq a$$
$$u = u^{(0)} = A \sin Kx + B \cos Kx$$

where

(2.27)
$$A = \left\{ u^{(i)}(a) \sin Ka + \frac{1}{K} u^{(i)\prime}(a) \cdot \cos Ka \right\}$$
$$B = \left\{ u^{(i)}(a) \cos Ka - \frac{1}{K} u^{(i)\prime}(a) \sin Ka \right\}$$

A and B are defined so that u is smooth across x = a. Clearly, since u has the form $u^{(o)}$ for x > a, the integrand of I is zero for x > a (see (2.16)) so that

$$(2.28)\qquad I = \int_0^a u^{(i)} \left\{ \frac{d^2}{dx^2} + \epsilon - V(x) \right\} u^{(i)}\, dx .$$

When (2.27) and (2.28) are substituted in (2.23), we have a variational principle involving only $u^{(i)}(x)$, whose asymptotic form no longer concerns us. The price paid, of course, is the reappearance of the cut-off distance a.

The Well-Depth as Proper Value.*

Before going on to a discussion of these methods let us note that if we write $V(x) = -\lambda f(x)$, where f(x) determines the shape and λ the depth of the potential well, we can regard λ as the proper value in the Schroedinger equation

$$(2.29)\qquad \left\{ \frac{d^2}{dx^2} + \kappa^2 + \lambda f(x) \right\} u(x) = 0 .$$

λ, as calculated from the equation,

$$(2.30)\qquad \int_0^\infty u(x) \left\{ \frac{d^2}{dx^2} + \kappa^2 + \lambda f(x) \right\} u(x) = 0$$

is stationary if

$$(2.31)\qquad \delta u(0) = 0 , \quad \delta u(\infty) = 0 .$$

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* This idea was used in connection with bound state problems by Svartholm (ref. 28).

Both K and η are now regarded as known while the strength of the interaction is the unknown. This is in contrast to methods 1-3 in which the interaction was regarded as given and K and η or K and L were determined as functions of one another.

While this approach has no advantages in connection with the Rayleigh-Ritz method, it provides a useful viewpoint in the variation iteration method to be discussed later (section II.8.).

Connection between Methods 1-3:

Methods 1 and 2 differ only with respect to which of the quantities L and K^2 is presumed known and which is unknown. With the same trial function and the same a they must lead to the same relation between $\tan\eta$ and K.

On the other hand method 3 differs slightly from 1 and 2. Let us trace the connection between the cut-off independent form of method 3 and method 2:

In the latter, L is determined from (2.5), which after an integration by parts gives

$$(2.32) \quad -u\frac{du}{dx}\Big|_{x=a} + I + L\,u^2(a) = 0$$

where I is defined by(2.28). If u has the asymptotic form (2.22)we can evaluate the two boundary terms, which leads to

$$-\frac{A^2}{\cos^2\eta_*} K \sin(Ka+\eta_*)\cos(Ka+\eta_*) + I$$

(2.33)

$$+\frac{A^2}{\cos^2\eta_*} K \cot(Ka+\eta)\sin^2(Ka+\eta_*) = 0,$$

where $\eta_* = \tan^{-1}(B/A)$. Multiplying (2.33) by $\frac{\cos^2\eta_*}{\sin^2(Ka+\eta_*)}$ we obtain

$$A^2 K\{\cot(Ka+\eta) - \cot(Ka+\eta_*)\} +$$

(2.34)

$$+ I\frac{\cos^2\eta_*}{\sin^2(Ka+\eta_*)} = 0$$

At the particular cut-off distances where

$$Ka = \frac{2n+1}{2}\pi, \tag{2.35}$$

(2.34) becomes

$$I + A^2 K \tan\eta_* = A^2 K \tan\eta. \tag{2.36}$$

This agrees precisely with the result (2.23) of method 3.

We now ask how η as determined by method 2 varies with a for a given trial function u which has the correct asymptotic form but incorrect phase shift. In (2.34), let us use the abbreviations

$$z = Ka + \eta_*, \quad \delta\eta = \eta_* - \eta$$

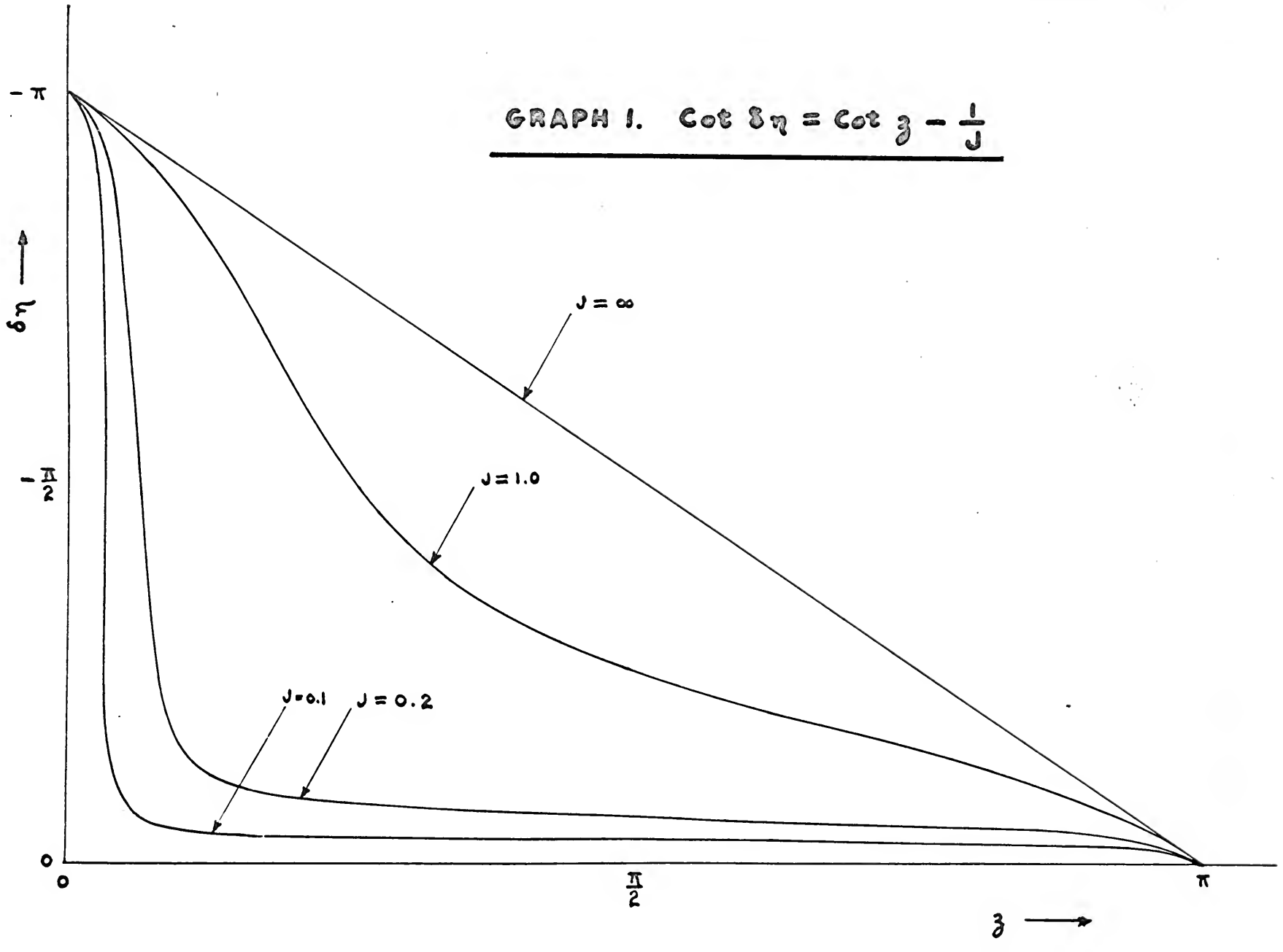
(2.37)

$$J = \frac{I}{A^2 K}\cos^2\eta_*$$

By some elementary manipulations we can then reduce it to

$$\cot\delta\eta = \cot z - 1/J. \tag{2.38}$$

For the correct wave function, J = 0, so that by (2.38)


GRAPH 1. Cot δη = Cot ȝ − 1/J
π
π/2
0
0
π/2
π
δη ⟶
ȝ ⟶
J = ∞
J = 1.0
J = 0.2
J = 0.1

$\delta\eta = 0$, except where $\cot z = \pm \infty$, that is where $ka + \eta_+ = n\pi$. At those points $\delta\eta$ is undefined. This is understandable from (2.5) since at those points $u = 0$ so that L is not determined.

The variation of $\delta\eta$ with z is shown for different values of J in Graph 1. For small values of J, cot z is negligible as compared to 1/J, except at the danger points $ka + \eta_+ = z = n\pi$, so that in the limit as $J \to 0$, $\delta\eta$ becomes independent of a.

Bilinear Formulation.

The Schroedinger variational principle for bound systems is usually stated in either of the two forms:

$$Q \equiv \int_0^\infty \left\{ -\left(\frac{du}{dx}\right)^2 - V(x)\,u^2 + \epsilon u^2 \right\} dx = 0 \qquad (2.39)$$

$$\delta Q = 0$$

or

$$Q \equiv \int_0^\infty u \left\{ \frac{d^2}{dx^2} - V(x) + \epsilon \right\} u \; dx = 0 \qquad (2.40)$$

$$\delta Q = 0$$

where all trial functions satisfy

$$\delta u(0) = 0 , \quad \delta u(\infty) = 0 . \qquad (2.41)$$

Let us recall that a modification of (2.39) for the case of a collision led to methods 1 and 2, while (2.40) was the starting point for method 3.

We can replace (2.39) and (2.40) by the following equivalent statements, involving bilinear instead of quadratic forms:

$$Q_{12} \equiv \int_0^\infty \left\{ -\left(\frac{du_1}{dx}\right)\left(\frac{du_2}{dx}\right) - V(x)\, u_1 u_2 + \epsilon u_1 u_2 \right\} dx = 0 \tag{2.42}$$

$$\delta Q_{12} = 0$$

or

$$Q_{12} = \int_0^\infty u_1 \left\{ \frac{d^2}{dx^2} - V(x) + \epsilon \right\} u_2 \, dx = 0 \tag{2.43}$$

$$\delta Q_{12} = 0$$

where all trial functions u_1 and u_2 satisfy

$$\delta u_i(0) = 0, \quad \delta u_i(\infty) = 0 \quad , \qquad i = 1, 2. \tag{2.44}$$

δ in (2.42) and (2.43) indicates independent variations of u_1 and u_2. The truth of (2.42) and (2.43) is directly verified from the Schroedinger equation and the boundary conditions (2.44).

Clearly the corresponding variational principles for collision problems can be similarly modified. Without going into details we shall merely state the results.

Methods 1 and 2:

$$J_{12} \equiv \int \left\{ -\left(\frac{du_1}{dx}\right)\left(\frac{du_2}{dx}\right) + k^2 u_1 u_2 - V(x)\, u_1 u_2 \right\} dx + L\, u_1(a)\, u_2(a) = 0 \tag{2.45}$$

$$\delta J_{12} = 0$$

if the trial functions satisfy

(2.46) $\delta u_i(0) = 0 \quad , \quad i = 1, 2 .$

(Compare to (2.5).)

Method 3:

(2.47) $K_{21} \equiv I_{21} + A_1 B_2 K - A_1 A_2 K \tan\eta = 0$

where $I_{21} = \int_0^\infty u_1 \left\{ \frac{d^2}{dx^2} + K^2 - V(x) \right\} u_2 \, dx$

(2.48) $\delta K_{21} = 0$

if the trial functions satisfy

(2.49) $$\left.\begin{aligned} &\delta u_i(0) = 0 \\ &u_i \longrightarrow A_i \sin Kx + B_i \cos Kx \end{aligned}\right\} \quad i = 1, 2 .$$

(Compare to (2.23), (2.24).) It is not at once apparent that $\tan\eta$ as calculated from (2.47) is symmetrical in u_1 and u_2. That this is so, however, follows from the fact that

$$I_{21} = \int_0^\infty u_1 \left\{ \frac{d^2}{dx^2} + K^2 - V(x) \right\} u_2 \, dx$$

(2.50) $$= \int_0^\infty u_2 \left\{ \frac{d^2}{dx^2} + K^2 - V(x) \right\} u_1 \, dx + \left(u_1 \frac{du_2}{dx} - u_2 \frac{du_1}{dx} \right)_{x=\infty}$$

$$= I_{12} + A_2 B_1 K - A_1 B_2 K .$$

In one dimensional problems there is no advantage in using the Rayleigh-Ritz method in conjunction with the bilinear variational principles instead of the quadratic ones. But we shall find the bilinear version useful in three

dimensional problems (sections I.4. - I.5.), where the Schroedinger equation has more than one solution, and in connection with the variation iteration method (sections II.8. - II.10.).

Numerical Illustrations.

Using the methods 2 and 3 we have calculated ^3S scattering of neutrons by protons at zero energy. We have assumed the interaction

$$V(x) = -4.01435 \qquad x \leq 1$$
$$= 0 \qquad x > 1 \tag{2.51}$$

(x measured in units of $r_0 = 2.80 \times 10^{-13}$ cm), which gives the correct binding energy for the deuteron. The wave equation, in this case, is simply

$$\frac{d^2u}{dx^2} + V(x)\,u = 0. \tag{2.52}$$

and can, of course, be solved exactly. For $x > 1$ the solution has the form $u = A\,(x + X)$ where X is the desired limiting ratio of $\tan \eta / K$, as K approaches zero.

As trial functions we have used

$$u_n = \sum_1^n c_l x^l \tag{2.53}$$

with n = 1, 2 and 3. Since (2.53) does not have the correct asymptotic form, it was necessary to use method 3 with a cut-off, a. The interaction vanishes at x = 1, which is the most appropriate choice for a. However to study the dependence of X on the cut-off distance, we have made calculations also for

larger values of a. Clearly a function of the form (2.53) can approximate the correct wave function better in a small than in a large interval, so that as a increases we expect our approximation for X to get worse.

The results are listed in Table I:

Table I.

Approximations to $X = \lim_{K \to 0} \tan\eta / K$.

$X_{exact} = -2.080$

a	$c_1 x$		$c_1 x + c_2 x^2$		$c_1 x + c_2 x^2 + c_3 x^3$	
	Method 2	Method 3	Method 2	Method 3	Method 2	Method 3
1	- 3.957	+ 1.338	- 2.112	- 2.126	- 2.083	- 2.084
2	+ 4.043	+ 1.338	- 2.858	- 4.039	- 2.201	- 2.206
3	+ 2.416	+ 1.338	- 6.593	- 51.606	- 2.385	- 2.520
4	+ 2.011	+ 1.338	+968.870	+ 7.634	- 2.936	- 3.315

These results exhibit a number of significant features:

1. The methods 2 and 3 lead to errors of the same order of magnitude. (In the present example method 2 is somewhat better.)

2. As expected, the results grow progressively worse with increasing a.

3. The dependence on a becomes weaker the larger the

number of parameters (except for the 1.338 column; see 5. below).

4. There appear singularities, owing to the wrong asymptotic behaviour of the trial functions. As the number of parameters increases the singularities move outwards, to infinity.

5. The trial function $c_1 x$, in method 3, leads to a result independent of a but of the wrong sign. This can be understood as follows: $c_1 x$ is the correct solution corresponding to no interaction. It has (accidentally) the correct asymptotic form (though wrong X) and therefore, by the theory of method 3, must lead to results independent of a. In fact we have

$$I = \int_0^a - V(x)\, u_1^2\, dx$$

(2.54)

$$A = \frac{1}{K} c_1, \quad B = 0,$$

all of which are independent of a. Using these in (2.23) we obtain for the determination of $X = \tan \eta / K$,

$$(2.55) \quad - \int_0^\infty V(x)\, u_1^2(x)\, dx = c_1^2 \tan \eta / K$$

which is precisely the Born approximation for $\tan \eta$. For small V the latter gives good results. But as V increases $(\tan \eta)_{Born}$ has a fixed sign while the true $\tan \eta$ eventually changes sign. This has occurred in our case, hence the wrong sign in the 1.338 - column.

In summary we may say:

(a) Method 1 is the least natural to collision problems.

(b) Method 2 appears to give slightly better results than method 3; but it suffers the aesthetic flaw of necessarily involving a cut-off distance.

(c) Method 3 is closely related to method 2. It does not necessarily involve a cut-off and yields the Born approximation for the phase shift as a special case.

(d) The Rayleigh-Ritz principle applied to either method 2 or 3 leads to a collision determinant instead of the usual secular determinant.

I.3. Variation of the Phase Shift with Energy. A Stationary Expression for the Width of a Resonance Level.

We have seen that methods 2 and 3 lead to stationary expressions for the phase shifts corresponding to arbitrary energies. It follows that it must also be possible to obtain a stationary expression for $d\eta/d\kappa^2$ which determines the variation of the scattering cross section with energy.

It is indifferent which of the two methods we use, but method 2 seems more convenient. We introduce the definition

$$(3.1)\quad M_K(u) \equiv \int_0^a \left[-\left(\frac{du}{dx}\right)^2 + \kappa^2 u^2 - V(x)u^2 \right] dx + L_\kappa u^2(a),$$

where L_K is the logarithmic derivative of the correct function u_K belonging to the energy K^2. By the Schroedinger equation (2.2), $M_K(u_K) = 0$, and by the stationary property,

(2.5), we have rigourously

$$M_K(u) = M_K(\delta u_K) = O(\delta u_K^2), \tag{3.2}$$

for any function $u = u_K + \delta u_K$. Differentiating (3.2) with respect to K we obtain, to the first order, in δu_K,

$$\frac{d\, M_K(u)}{d\, K} = 0 \tag{3.3}$$

Hence by (3.1), we find the equation

$$2K \int_0^a u^2\, dx + \frac{dL_K}{dK}\, u^2(a) = 0 \tag{3.4}$$

which is a stationary expression for dL_K/dK.

From this equation we can determine $d\eta/d(K^2)$ as follows. We note that

$$L_K = K \cot(Ka + \eta_K) \tag{3.5}$$

Hence

$$\frac{dL_K}{dK} = \cot(Ka+\eta_K) - \operatorname{cosec}^2(Ka+\eta_K)\left(Ka + K\frac{d\eta_K}{dK}\right) \tag{3.6}$$

so that

$$\frac{d\eta_K}{d(K^2)} = \frac{1}{2K}\,\frac{d\eta_K}{dK}$$

$$= \frac{dL_K}{dK}\,\frac{\sin^2(Ka+\eta_K)}{2K^2} + \frac{\sin\{2(Ka+\eta_K)\}}{4K^2} - \frac{a}{2K} \tag{3.7}$$

$$= \frac{\int_0^a u^2\, dx}{K\, u^2(a)} \cdot \sin^2(Ka+\eta_K) + \frac{\sin\{2(Ka+\eta_K)\}}{4K^2} - \frac{a}{2K}.$$

We may observe that this stationary expression for involves only the wave function and the correct phase shift η_K, while all reference to the interaction has disappeared.

Let us check that if $d\eta_K/d(K^2)$ is computed from (3.7), using the correct wave function u_K, the apparent dependence of $d\eta_K/d(K^2)$ on a disappears, as it must, as long as a exceeds the range of interaction, a_0.

For $x > a_0$, the correct u_K has the form

$$u_K(x) = C \sin(Ka + \eta_K) \tag{3.8}$$

Hence

$$\frac{d\eta_K}{d(K^2)} = \frac{1}{KC^2}\int_0^a u_K^2\,dx + \frac{\sin\{2(Ka+\eta_K)\}}{4K^2} - \frac{a}{2K}. \tag{3.9}$$

Differentiating with respect to a we find

$$\frac{\partial}{\partial a}\left(\frac{d\eta_K}{d(K^2)}\right) = \frac{1}{KC^2}\cdot C^2\cdot\sin^2(Ka+\eta_K) + \frac{\cos\{2(Ka+\eta_K)\}}{2K} - \frac{1}{2K}$$

(3.10)

$$= \frac{1}{2K}\left\{\cos\{2(Ka+\eta_K)\} + 2\sin^2(Ka+\eta_K) - 1\right\}$$

$$= 0$$

which proves that $d\eta/d(K^2)$ is independent of a.

As an application of (3.7) we shall derive a stationary expression for the level width at resonance.

In the neighbourhood of a resonance energy, defined by the condition that $\eta_K = (n+\frac{1}{2})\pi$, $\tan\eta_K$ has a singularity of the form

$$\tan \eta_K = \frac{\frac{1}{2}\Gamma}{K^2 - K_\lambda^2} \,, \tag{3.11}$$

where K_λ^2 is the resonance energy. Γ is called the level width because the cross section in the vicinity of K_λ is given by

$$\sigma = \frac{4\pi}{K^2} \frac{\left(\frac{1}{2}\Gamma\right)^2}{\left(K^2 - K_\lambda^2\right)^2 + \left(\frac{1}{2}\Gamma\right)^2} \tag{3.12}$$

Now near K_λ,

$$\eta_K = \left(n + \tfrac{1}{2}\right)\pi + \frac{d\eta_K}{d\left(K_\lambda^2\right)} \left(K^2 - K_\lambda^2\right). \tag{3.13}$$

Therefore

$$\tan \eta_K = - \frac{1 \Big/ \frac{d\eta_K}{d\left(K_\lambda^2\right)}}{K^2 - K_\lambda^2} \,. \tag{3.14}$$

Hence, comparing (3.11) and (3.14) and using (3.9) with $\eta = \left(n + \frac{1}{2}\right)\pi$, we find the following stationary expression for $\frac{1}{2}\Gamma$:

$$\frac{1}{2}\Gamma = - \frac{1}{\frac{d\eta_K}{d\left(K_\lambda^2\right)}} \tag{3.15}$$

$$= \frac{4K_\lambda^2}{- \frac{4K_\lambda}{u^2(a)} \cos^2 Ka \int_0^a u^2 dx + 2aK - \sin(2aK)}$$

I.4. A Variational Principle for the Scattering Amplitude.

When dealing with a wave function of given angular momentum, a correspondence to a bound state problem can be established because we know, a priori, that asymptotically the solution has a radial logarithmic derivative independent of the angle. But if we want to treat the whole incident plane wave at once no such information is available. We have already seen that only method 3 need not involve an enclosure and that the Born approximation for individual phases can be deduced from it. Both facts suggest that it would be the most promising attack on the scattering amplitudes of three dimensional problems.

The wave equation for the relative motion of two colliding particles of equal mass M is

$$\left\{-\frac{\hbar^2}{M}\nabla^2 + U(R)\right\}\Psi(R) = E\,\Psi(R), \tag{4.1}$$

where R is their relative position vector and U (R) is the interaction potential. Setting

$$r = \frac{R}{\lambda_0}\,,\quad \kappa^2 = \frac{ME}{\hbar^2}\lambda_0^2\,,\quad V(r) = \frac{MU(\lambda_0 r)}{\hbar^2}\lambda_0^2$$

$$\psi(r) = \Psi(\lambda_0 r)\,, \tag{4.2}$$

where λ_0 is our unit of length, it becomes

$$(4.3)\qquad \left\{\nabla^2 + \kappa^2 - V(r)\right\}\psi(r) = 0$$

We shall now follow a procedure corresponding to the bilinear form of method 3 (see (2.47) - (2.49)). We define ψ_{-K_1}, and ψ_{K_2} as the two solutions of (4.3) which correspond to plane waves incident along $-K_1$ and K_2 and have the asymptotic forms

$$(4.4)\qquad \begin{aligned} \psi_{-K_1} &\longrightarrow e^{-iK_1\cdot r} + f(-K_1, K)\,\frac{e^{i\kappa r}}{r}, \\ \psi_{K_2} &\longrightarrow e^{iK_2\cdot r} + f(K_2, K)\,\frac{e^{i\kappa r}}{r}. \end{aligned}$$

Here $|K_1| = |K_2| = |K|$ and $f(K_i, K)$ is the scattering amplitude in the direction K of a wave incident along K_i. Corresponding to (2.47) we now define

$$(4.5)\qquad I_{K_2, K_1} = \int_0 \psi_{-K_1}\left(\nabla^2 + \kappa^2 - V\right)\psi_{K_2}\,(dr).$$

In virtue of (4.3), we find after an integration by parts,

$$(4.6)\qquad \delta I_{K_2, K_1} = \int_S \left\{\psi_{-K_1}\frac{\partial}{\partial n}\delta\psi_{K_2} - \delta\psi_{K_2}\frac{\partial}{\partial n}\psi_{-K_1}\right\} dS$$

where S is a large sphere, and $\frac{\partial}{\partial n}$ denotes differentiation along the outward normal.

Now let us admit only trial functions of the asymptotic form (4.4), but with possibly incorrect f's, so that asymptotically

$$(4.7)\qquad \delta\psi_{K_2} \longrightarrow \delta f^{(n)}(K_2, K)\,\frac{e^{i\kappa r}}{r}.$$

where $\delta f^{(2)}(K_2, K)$ is the error in the scattering amplitude of the trial function ψ_{K_2}. Clearly only the plane wave part of ψ_{K_1} contributes to the surface integral (4.6) so that

$$\delta I_{K_2,K_1} = \int_S \left\{ e^{-iK_1\cdot r} \frac{\partial}{\partial n} \frac{e^{iKr}}{r} - \frac{e^{iKr}}{r} \frac{\partial}{\partial n} e^{-iK_1\cdot r} \right\} \delta f^{(2)}(K_2, K)\, dS. \tag{4.8}$$

Dirac [37] has shown that the factor multiplying $\delta f^{(2)}(K_2 K)$ has a δ - function like character for large values of r, so that the integration gives simply

$$\delta I_{K_2,K_1} = -\, 4\pi\, \delta f^{(2)}(K_2, K_1). \tag{4.9}$$

Since for the correct ψ_{K_2}, $I_{K_2,K_1} = 0$, it follows that $f(K_2, K_1)$, as calculated from the equation

$$I_{K_2,K_1} + 4\pi f^{(2)}_{trial}(K_2, K_1) = 4\pi f(K_2, K_1) \tag{4.10}$$

is stationary with respect to independent variations of ψ_{-K_1} and ψ_{K_2}, subject to the conditions (4.7).

Symmetry Properties.

Equation (4.10) involves two trial function, ψ_{-K_1} and ψ_{K_2}. These differ by a rotation in the coordinate space

37. P. A. M. Dirac, The Principles of Quantum Mechanics, (Clarendon Press, Oxford 1947), third ed., p. 191.

and, in general, also in their functional form (to the first order). Let us indicate the functional form by superscripts and write explicitly $\psi^{(1)}_{-K_1}$, $\psi^{(2)}_{K_2}$ for our trial functions, and $f^{(i,j)}(K_2, K_1)$ for the f obtained from (4.10) by using $\psi^{(i)}_{-K_1}$ first and $\psi^{(j)}_{K_2}$ second in (4.5). Integrations by parts, analogous to (2.50), reveal the following symmetry properties which are not at once apparent from (4.10):

$$f^{(1,2)}(K_2, K_1) = f^{(2,1)}(K_2, K_1), \tag{4.11}$$

$$f^{(1,2)}(-K_2, K_1) = f^{1,2}(-K_1, K_2). \tag{4.12}$$

(4.11) implies that f is invariant under interchange of the functional forms of ψ_{-K_1}, and ψ_{K_2}, as will be verified below in the case of the Born approximations. (4.12) guarantees that the scattering kernel $f(-K_2, K_1)$ is symmetrical when computed by (4.10).

Connection with Born Approximations.

The simplest admissible trial functions are

$$\psi_{-K_1} = e^{-iK_1\cdot r}, \qquad \psi_{K_2} = e^{iK_2\cdot r}. \tag{4.13}$$

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38. Ref. 18, eq. (2.52).

Substituting these in (4.10) we obtain

$$(4.14)\quad -\int e^{-i\mathbf{K}_1\cdot\mathbf{r}}\, V\, e^{i\mathbf{K}_2\cdot\mathbf{r}} = 4\pi f(\mathbf{K}_2, \mathbf{K}_1)$$

which is identical with the result of the first Born approximation.

We obtain the second Born approximation if we use one first Born approximation trial function and one plane wave; i.e. either

$$(4.15)\quad \psi_{-\mathbf{K}_1} = \psi^{(1)}_{-\mathbf{K}_1} \equiv e^{-i\mathbf{K}_1\cdot\mathbf{r}}$$

$$\psi_{\mathbf{K}_2} = \psi^{(2)}_{\mathbf{K}_2} \equiv e^{i\mathbf{K}_2\cdot\mathbf{r}} - \int \frac{e^{iK|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}')\, e^{i\mathbf{K}_2\cdot\mathbf{r}'}\, (d\mathbf{r}')$$

or

$$(4.16)\quad \psi_{-\mathbf{K}_1} = \psi^{(2)}_{-\mathbf{K}_1}$$

$$\psi_{\mathbf{K}_2} = \psi^{(1)}_{\mathbf{K}_2}$$

in agreement with (4.11). Higher Born approximations are obtained in a similar way.

Thus, apart from re-deducing the Born approximations from a variational principle, nothing new is gained by using these iterated functions in (4.10).

Application of the Rayleigh-Ritz Method.

We can use the Rayleigh-Ritz Method in conjunction with (4.10) to determine the scattering amplitude $f(\mathbf{K}_2, \mathbf{K}_1)$

This is analogous to method 3 (section I.2.) for calculating the tangent of the phase shift. For simplicity, we use the same functional form for ψ_{-K_1} and ψ_{K_2} and write

$$\psi_{-K_1} = c_1 e^{-i K_1 \cdot r} + c_2 u_{-K_1;2} + \cdots c_n u_{-K_1;n},$$

(4.17)

$$\psi_{K_2} = c_1 e^{i K_2 \cdot r} + c_2 u_{K_2;2} + \cdots c_n u_{K_2;n},$$

where the trial functions $u_{K;i}$ have the asymptotic form

$$u_{K;i}(r) \longrightarrow f_i(K, K') \frac{e^{iK'r}}{r} \qquad (4.18)$$

Clearly for use with trial functions of the form (4.17) instead of (4.4), (4.10) must be replaced by the equivalent homogeneous equation

$$I_{K_2,K_1} + 4\pi c_1 \sum_{i=2}^{n} c_i f_i(K_2, K_1) = 4\pi c_1^2 f(K_2, K_1), \qquad (4.19)$$

where I_{K_2,K_1} is defined by (4.5).

When (4.19) is written out in terms of the trial functions it assumes the form

$$\sum_{\substack{i=1 \\ j=1}}^{n} A_{ij} c_i c_j = 4\pi f(K_2, K_1) c_1^2 \qquad (4.20)$$

where we may take $A_{ij} = A_{ji}$. The stationary property of f relative to variations of the c_i then leads to the equations

$$\sum_{j=1}^{n} A_{1j} c_j = 4\pi f(K_2, K_1) \cdot c_1$$

$$\sum_{j=1}^{n} A_{ij} c_j = 0 \quad , \qquad i = 2, \ldots n. \qquad (4.21)$$

They are compatible only if the determinant of the coefficients vanishes, that is if

$$(4.22)\quad \Delta(K_2,K_1) \equiv \begin{vmatrix} A_{11}-4\pi f(K_2,K_1) & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{vmatrix} = 0$$

$f(K_2, K_1)$ is uniquely defined by (4.22). The fact that it is, in general, complex is reflected by the collision determinant $\Delta(K_2 K_1)$ whose matrix is symmetrical but not hermitian.

On varying the angle between $-K_1$ and K_2 one can obtain stationary expressions for the scattering amplitudes, and hence for the differential cross section, in all directions.

I.5. Non-Central Forces.

It is well known that if two particles interact by means of a potential which depends only on their distance of separation, the relative angular momentum is conserved. This fact is the basis of the phase method in collision problems, whose variational formulation has been discussed in sections I.2. and I.3.

However, the hypothesis that nuclear forces are purely central is untenable in view of the quadrupole moment of the deuteron, and has been replaced by the assumption that they are a mixture of central and non-central forces. Rarita and

Schwinger[3] have worked out the combinatorial aspects introduced into the 2-body problem by the existence of such non-central, so-called tensor forces. In particular they have shown that the angular momentum is no longer conserved, and that the eigenstates of the Hamiltonian, instead of being S, P, D,.... states are now, in general, mixtures of such states. Most important, in the neutron-proton system at low energies, is the S + D mixture.

In our method of section I.4., the conservation of angular momentum did not have to be assumed and thus it applies without change to collisions involving tensor forces. This method deals with all angular momenta at once. It may however be desirable to treat each eigenstate separately. This can be done in a way related both to the three dimensional procedure of section I.4. and to either method 2 or 3 of section I.2.

As mentioned above, it has been shown from the transformation properties of the Hamiltonian that there are solutions of the Schroedinger equation consisting of mixtures of S and D states. These solutions are proper functions of the Hamiltonian, H; the total angular momentum J; its z-component J_z ; the total spin S; and the parity operator, P. In the scattering of neutrons by protons the incident plane wave includes both S and D waves in which these operators have the same proper values. The amplitudes, β_S , β_D of the outgoing S and D waves are related to the amplitudes α_S , α_D of the incoming waves by a unitary, symmetrical scattering matrix S. Thus

(5.1) $$\beta = S \cdot \alpha$$

where

$$\alpha = \begin{pmatrix} \alpha_S \\ \alpha_D \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_S \\ \beta_D \end{pmatrix}$$

(5.2)
$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}.$$

We know α_S and α_D. To find the differential cross section we must determine the elements S_{ij} which give β_S and β_D by (5.1). Actually it is sufficient to determine two of the (complex) elements S_{ij} since due to its symmetry and unitary character,[39] the matrix S involves only three independent constants.

Consider the expression

(5.3) $$I_{21} = \int \psi^{(1)} \left(\nabla^2 + K^2 - V \right) \psi^{(2)} \, (dr),$$

where $\psi^{(1)}$ and $\psi^{(2)}$ are the solutions of the Schroedinger equation,

(5.4) $$\left(\nabla^2 + K^2 - V \right) \psi = 0,$$

which have the asymptotic form

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39. See ref. (18).

$$\psi^{(2)} \longrightarrow \left\{ \alpha_S^{(2)} \frac{e^{-i\kappa r}}{r} + \beta_S^{(2)} \frac{e^{i\kappa r}}{r} \right\} \Omega_S + \left\{ \alpha_D^{(2)} \frac{e^{-i\kappa r}}{r} + \beta_D^{(2)} \frac{e^{i\kappa r}}{r} \right\} \Omega_D$$

$$\psi^{(1)} \longrightarrow \left\{ \alpha_S^{(1)} \frac{e^{-i\kappa r}}{r} + \beta_S^{(1)} \frac{e^{i\kappa r}}{r} \right\} \Omega_S^* + \left\{ \alpha_D^{(1)} \frac{e^{-i\kappa r}}{r} + \beta_D^{(1)} \frac{e^{i\kappa r}}{r} \right\} \Omega_D^* . \tag{5.5}$$

Here Ω_S, Ω_D describe the normalized angular and spin functions of the S and D wave respectively. Now let us use, in (5.3), trial functions whose asymptotic variation is

$$\delta\psi^{(2)} \longrightarrow \delta\beta_S^{(2)} \frac{e^{i\kappa r}}{r} \Omega_S + \delta\beta_D^{(2)} \frac{e^{i\kappa r}}{r} \Omega_D$$

$$\delta\psi^{(1)} \longrightarrow \delta\beta_S^{(1)} \frac{e^{i\kappa r}}{r} \Omega_S^* + \delta\beta_D^{(1)} \frac{e^{i\kappa r}}{r} \Omega_D^* . \tag{5.6}$$

Then

$$\delta I_{21} = \int \left\{ \psi^{(1)} \frac{\partial}{\partial n} \delta\psi^{(2)} - \delta\psi^{(2)} \frac{\partial}{\partial n} \psi^{(1)} \right\} dS$$

$$= 2ik \left\{ \alpha_S^{(1)} \cdot \delta\beta_S^{(2)} + \alpha_D^{(1)} \delta\beta_D^{(2)} \right\} \tag{5.7}$$

Hence, to the first order, we have

$$I_{21} + \frac{2k}{i} \left[\alpha_S^{(1)} \beta_{S,\,trial}^{(2)} + \alpha_D^{(1)} \beta_{D,\,trial}^{(2)} \right]$$

$$= \frac{2k}{i} \left[\alpha_S^{(1)} \beta_S^{(2)} + \alpha_D^{(1)} \beta_D^{(2)} \right] ; \tag{5.8}$$

or, in the matrix notation of (5.2)

$$I_{21} + \frac{2k}{i} \alpha^{(1)} \cdot \beta^{(2)}{}_{,\,trial} = \frac{2k}{i} \alpha^{(1)} \cdot \beta^{(2)}$$

$$= \frac{2k}{i} \alpha^{(1)} \cdot S \cdot \alpha^{(2)} . \tag{5.9}$$

This enables us to obtain all matrix elements S_{ij}. For example, to find S_{12} we use trial functions with $\alpha_D^{(1)}=0$, $\alpha_S^{(2)}=0$ in which case the right hand side of (5.9) becomes

$$(5.10)\qquad \frac{2K}{i}\begin{pmatrix}\alpha_S^{(1)} & 0\end{pmatrix}\begin{pmatrix}S_{11} & S_{12}\\ S_{21} & S_{22}\end{pmatrix}\begin{pmatrix}0\\ \alpha_D^{(2)}\end{pmatrix}=\frac{2K}{i}\alpha_S^{(1)}\alpha_D^{(2)}S_{12},$$

and an application of the Rayleigh-Ritz method will yield the required matrix element.

Let us note here that in this way we obtain a stationary result for the differential as well as for the total cross section (The stationary character of the differential cross section is lost in the method of proper phases, described below.)

The Structure of the Collision Determinant.

Suppose we want to calculate the element S_{11} by the Rayleigh-Ritz method. We use as trial functions

$$\Psi_t^{(1)}=\left\{\alpha_S^{(1)}\frac{e^{-iKr}}{r}+\beta_{S,\,trial}^{(1)}\frac{e^{iKr}}{r}+S_1^{(1)}u_1^{(1)}+S_2^{(1)}u_2^{(1)}+\dots\right\}\Omega_S^*$$

$$+\left\{\beta_{D,\,trial}^{(1)}\frac{e^{iKr}}{r}+d_1^{(1)}w_1^{(1)}+d_2^{(1)}w_2^{(1)}+\dots\right\}\Omega_D^*$$

$$(5.11)\qquad \Psi_t^{(2)}=\left\{\alpha_S^{(2)}\frac{e^{-iKr}}{r}+\beta_{S,\,trial}^{(2)}\frac{e^{iKr}}{r}+S_1^{(2)}u_1^{(2)}+S_2^{(2)}u_2^{(2)}+\dots\right\}\Omega_S$$

$$+\left\{\beta_{D,\,trial}^{(2)}\frac{e^{iKr}}{r}+d_1^{(2)}w_1^{(2)}+d_2^{(2)}w_2^{(2)}+\dots\right\}\Omega_D.$$

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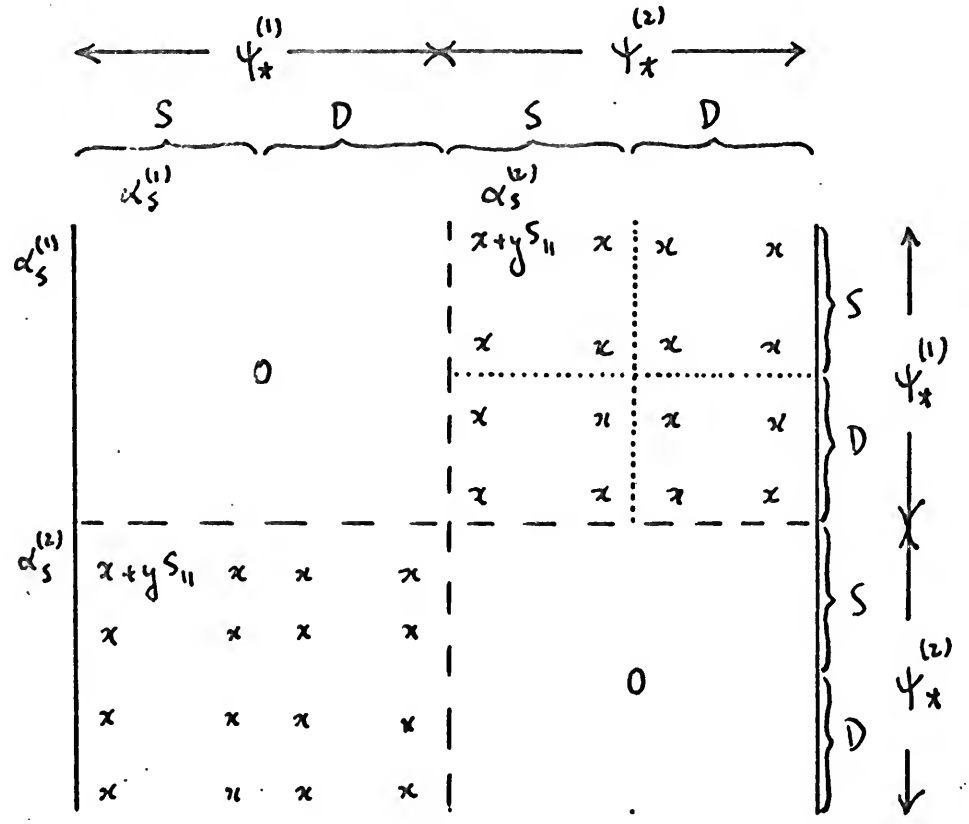
40. For calculating S_{11} we need not use different functional

where the radial functions $u^{(i)}$ and $w^{(i)}$ vanish rapidly as $r \longrightarrow \infty$. Thus each trial function consists of an S and a D part. Using the functions (5.11) in (5.9) we find that the tensor character of the potential introduces elements connecting all coefficients of $\psi_\pi^{(1)}$ with those of $\psi_\pi^{(2)}$. The unknown S_{II} is introduced by the right hand side of (5.9) and occurs only as factor of $\alpha_S^{(1)}\,\alpha_S^{(2)}$.

On using the stationary property of S_{II}, we are led to a system of equations precisely as in section I.2. These are compatible only if the determinant of the coefficients, Δ_{II}, vanishes. In the present case Δ_{II} has clearly the following, symmetrical form:

(5.12)

$$\Delta_{II} =$$



forms for $\psi_\pi^{(1)}$ and $\psi_\pi^{(2)}$. We use them here because for calculating off-diagonal elements of S, different functional forms obviously are required.

Because of its symmetry $\Delta_{11} = \pm(\Delta'_{11})^2$, where Δ'_{11} is the large upper right hand block of Δ_4. S_{11} is therefore determined by the linear equation $\Delta_4' = 0$. Δ_4' comprises two blocks of elements connecting S and D functions. These describe the interaction between the S and D state. In the limiting case of vanishing tensor forces they become zero and Δ_{11}' assumes the degenerate form

(5.13)
$$\Delta_{11}' \longrightarrow \begin{array}{c} \overbrace{}^{S} \quad \overbrace{}^{D} \\ \left|\begin{array}{cccc} x+yS_{11} & x & 0 & 0 \\ x & x & 0 & 0 \\ 0 & 0 & x & x \\ 0 & 0 & x & x \end{array}\right| \end{array} \begin{array}{l} \} S \\ \\ \} D \\ \\ \end{array}$$

Hence S_{11} is determined from the equation

(5.14)
$$\begin{array}{c} \overbrace{}^{S} \\ \left|\begin{array}{cc} x+yS_{11} & x \\ x & x \end{array}\right| \end{array} \begin{array}{l} \} S \\ \\ \end{array} = 0.$$

whose elements no longer involve any D functions. This expresses the fact that the S wave is now decoupled from the D wave. In fact (5.14) has the same structure as (2.14), which was arrived at by considering only the S waves.

Proper Values of the Scattering Matrix.

The unitary matrix S has two eigenstates $\varphi^{(I)}$ and $\varphi^{(II)}$ with the property that

$$\beta^{(i)} \equiv S \cdot \alpha^{(i)} = \chi^{(i)} \alpha^{(i)} \quad \text{(not summed)} \tag{5.15}$$

$$i = I, II.$$

The $\chi^{(i)}$ are the proper values of S and, because of its unitary character, may be written as

$$\chi^{(I)} = -e^{2i\eta_I} \quad , \quad \chi^{(II)} = -e^{2i\eta_{II}}. \tag{5.16}$$

Thus the eigenstates have the asymptotic form

$$\begin{aligned} \varphi^{(I)} \longrightarrow\ & \alpha_S^{(I)} \left(\frac{e^{-ikr}}{r} - e^{2i\eta_I} \frac{e^{ikr}}{r} \right) \Omega_S \\ & + \alpha_D^{(I)} \left(\frac{e^{-ikr}}{r} - e^{2i\eta_I} \frac{e^{ikr}}{r} \right) \Omega_D \end{aligned} \tag{5.17}$$

$$= -2i\, e^{i\eta_I} \cdot \sin(kr + \eta_I)\left(\alpha_S^{(I)} \Omega_S + \alpha_D^{(I)} \Omega_D\right).$$

$$\varphi^{(II)} \longrightarrow -2i\, e^{i\eta_{II}} \cdot \sin(kr + \eta_{II})\left(\alpha_S^{(II)} \Omega_S + \alpha_D^{(II)} \Omega_D\right). \tag{5.18}$$

$\varphi^{(I)}$ and $\varphi^{(II)}$ are thus standing waves with real radial functions and for that reason they are simpler to deal with than other states which are, in general, complex linear combinations of $\varphi^{(I)}$ and $\varphi^{(II)}$. Furthermore Schwinger[41] has shown that the

41. J. Schwinger, unpublished lectures.

total cross section of the S + D mixture of a plane wave can be expressed in terms of the two constants η_I and η_{II} only, namely

$$\sigma = \frac{4\pi}{k^2}\left(\sin^2\eta_I + \sin^2\eta_{II}\right) \tag{5.19}$$

It is therefore of interest that $\tan\eta_I$ and $\tan\eta_{II}$ can be directly obtained by our method. In fact this problem is very much akin to that of finding $\tan\eta$ in the case of central forces (section I.2.).

We could proceed from the most general equation (5.9) but the following approach is slightly simpler:

The correct $\varphi^{(I)}$ and $\varphi^{(II)}$ both have the form

$$\varphi = \left\{a_1 \frac{\sin kr}{r} + a_2 \frac{\cos kr}{r} + a_3 u_3 + \dots\right\}\Omega_S + \left\{b_1 \frac{\sin kr}{r} + b_2 \frac{\cos kr}{r} + b_3 w_3 + \dots\right\}\Omega_D, \tag{5.20}$$

where the a_λ, b_λ, u_λ and w_λ may be taken as real and $\frac{a_2}{a_1} = \frac{b_2}{b_1} = \tan\eta_{I\text{ or }II}$.

Consider now the expression

$$I = \int \varphi^* \left(\nabla^2 + k^2 - V\right)\varphi\,(dr) \tag{5.21}$$

where we admit only such trial-φ's, whose variations have the asymptotic form

$$\delta\varphi \to \left\{\delta a_1 \frac{\sin kr}{r} + \delta a_2 \frac{\cos kr}{r}\right\}\Omega_S + \left\{\delta b_1 \frac{\sin kr}{r} + \delta b_2 \frac{\cos kr}{r}\right\}\Omega_D. \tag{5.22}$$

Proceeding in the usual way, one finds

$$\delta I = \int \left\{ \varphi^* \frac{\partial}{\partial n} \varphi - \delta\varphi \frac{\partial}{\partial n} \varphi^* \right\} ds$$

(5.23)

$$= -K \left\{ a_1^2 \, \delta\left(\frac{a_2}{a_1}\right) + b_1^2 \, \delta\left(\frac{b_2}{b_1}\right) \right\}.$$

Therefore, corresponding to (2.23), we find

$$I + K\left(a_1 a_2 + b_1 b_2\right) = K\left(a_1^2 + b_1^2\right) \tan\eta \qquad (5.24)$$

as a stationary expression for $\tan \eta_{I \text{ or } II}$.

When we substitute a trial function of the form (5.20) in (5.24) we obtain an equation of the type

$$\sum_{i,j} \left\{ P_{ij} \, a_i a_j + Q_{ij} \, a_i b_j + R_{ij} \, b_i b_j \right\} = K\left(a_1^2 + b_1^2\right) \tan\eta. \qquad (5.25)$$

Proceeding in the usual way to a set of linear equations and their compatibility condition we find the following determinantal equation for $\tan \eta$:

$$\Delta = \qquad (5.26)$$

	S		D	
S	$P_{11} - K\tan\eta$	$P_{12} \ldots$	Q_{11}	$Q_{12} \ldots$
	P_{21}	$P_{22} \ldots$	Q_{21}	$Q_{22} \ldots$
	⋮	⋮	⋮	⋮
D	Q_{11}	$Q_{21} \ldots$	$R_{11} - K\tan\eta$	$R_{12} \ldots$
	Q_{12}	$Q_{22} \ldots$	R_{21}	$R_{22} \ldots$
	⋮	⋮	⋮	⋮

$= 0$

Clearly this is a quadratic equation for $\tan\eta$, yielding approximations for $\tan\eta_I$ and $\tan\eta_{II}$. The elements Q_{ij} arise from the interaction of S and D functions. In the absence of tensor forces they vanish so that Δ factors and we are led back to two independent problems for the S and D wave (compare (2.14)).

From the two solutions for $\tan\eta$ we can find the total cross section by (5.18), whose error will be of the second order if our trial wave function has a first order error. We can also find the differential cross section to the same order of accuracy as our trial function by solving the linear equations derived from (5.25) for the a_i and b_i, thus obtaining the wave functions $\varphi^{(I)}$ and $\varphi^{(II)}$ and then taking that linear combination whose incident wave agrees with the incident S and D waves contained in a plane wave. To obtain the differential cross section to the second order of accuracy, we must fall back on the more general but more complicated equation (5.9).

Numerical Illustration.

By using the method of proper values of the scattering matrix, we have calculated $\tan\eta_I$ and $\tan\eta_{II}$ for neutron-proton $^3S_1 + {}^3D_1$ scattering at 2.82 MEV. We have used the constants of Rarita and Schwinger [3] to have a comparison with Schwinger's numerical integration [41] for the same energy. Thus the following interaction potential was used:

$$(5.27)\qquad V = \lambda\left\{ f(r) + 2^{-3/2} g(r) S_{12}\right\},$$

where

$$\lambda = 2.62828$$

$$f(r) = -1 \quad , \quad r \leq 1$$

$$= 0 \quad , \quad r > 1 \tag{5.28}$$

$$g(r) = -2.19203 \quad , \quad r \leq 1$$

$$= 0 \qquad\quad r > 1$$

and S_{12} is the spin dependent tensor operator,

$$S_{12} = 3\,\frac{(\sigma_1 \cdot r)(\sigma_2 \cdot r)}{r^2} - \sigma_1 \cdot \sigma_2 \tag{5.29}$$

r is measured in units of $\lambda_0 = 2.80 \times 10^{-13}$ cm.

Schwinger[3] has shown that the Schroedinger equation leads, in the present case, to two coupled equations for the radial functions $u(r)$ and $w(r)$ of the S and D wave, viz.

$$\left(\frac{d^2}{dr^2} + K^2\right) u + \lambda\left(f u + g w\right) = 0 \tag{5.30}$$

$$\left(\frac{d^2}{dr^2} - \frac{6}{r^2} + K^2\right) w + \lambda\left(g u + h w\right) = 0 , \tag{5.31}$$

where f and g are defined in (5.28) and $h = 1 - 2^{1/2} g$. It is simpler to base our variational procedure on these equations, rather than to go back to the original three

dimensional Schroedinger equation. We define

$$I = \int_0^\infty \{ u \left[\left(\frac{d^2}{dr^2} + K^2 \right) u + \lambda \left(f u + g w \right) \right] + w \left[\left(\frac{d^2}{dr^2} + K^2 - \frac{b}{r^2} \right) w + \lambda \left(g u + h w \right) \right] \} \, dr . \tag{5.32}$$

If we use trial functions with the asymptotic form

$$u \longrightarrow A_S \left(\sin Kr + \tan \eta_*^{(S)} \cos Kr \right)$$
$$w \longrightarrow -A_D \left(\sin Kr + \tan \eta_*^{(D)} \cos Kr \right) \tag{5.33}$$

we find

$$\delta I = \left(u \frac{d}{dr} \delta u - \delta u \frac{d}{dr} u \right) + \left(w \frac{d}{dr} \delta w - \delta w \frac{d}{dr} w \right)$$
$$= -K \left(A_S^2 \delta \tan \eta^{(S)} + A_D^2 \, \delta \tan \eta^{(D)} \right). \tag{5.34}$$

Now the exact solutions which we are looking for have $\tan \eta_S = \tan \eta_D = \tan \eta$. Hence the equation

$$I + K \left(A_S^2 \tan \eta_*^{(S)} + A_D^2 \tan \eta_*^{(D)} \right)$$
$$= K \left(A_S^2 + A_D^2 \right) \tan \eta_1 \tag{5.35}$$

where "t" indicates the trial function as usual, gives a stationary expression for $\tan \eta$.

We have used as trial functions

$$
\left.
\begin{aligned}
u_n &= \sum_1^n c_k r^k \qquad n = 1, 2, 3 \\
w_m &= \sum_1^m d_k r^{k+2} \qquad m = 1, 2
\end{aligned}
\right\} \quad r \leq 1 \tag{5.36}
$$

A_S, A_D, $\tan \eta_*^{(S)}$ and $\tan \eta_*^{(D)}$ were determined from the requirement that at $r = 1$ the functions (5.36) pass smoothly into the free particle functions

$$
\left.
\begin{aligned}
u &= A_S \left(\sin Kr + \tan \eta_*^{(S)} \cdot \cos Kr \right) \\
w &= -A_D \left(-j_2(Kr) + \tan \eta_*^{(D)} n_2(Kr) \right)
\end{aligned}
\right\} \quad r > 1 \tag{5.37}
$$

As checks on our calculation we have at each stage computed, by the variational method, the S and D phase shifts when tensor forces are absent and compared the results with the exact values which are easily obtained for the uncoupled states. The results of our calculations are collected in Table II.

Table II.

S + D Scattering with Tensor Forces.

Trial Functions	Uncoupled		Coupled	
	$\tan\eta^{(S)}$	$\tan\eta^{(D)} \times 10^4$	$\tan\eta_I$	$\tan\eta_{II}$
$u = c_1\lambda + c_2\lambda^2$ $w = d_1\lambda^3$	6.9850	- 0.3199	6.986	- 0.0003
$u = c_1\lambda + c_2\lambda^2$ $w = d_1\lambda^3 + d_2\lambda^4$	6.9850	- 0.3070	- 1.525	- 0.0002
$u = c_1\lambda + c_2\lambda^2 + c_3\lambda^3$ $w = d_1\lambda^3 + d_2\lambda^4$	9.1398	- 0.3070	- 1.425	- 0.0002
Correct Functions	9.2314	- 0.3069	- 1.435	0.0000

It is seen that the last pair of trial functions gives good agreement with Schwinger's numerical integration.

I.6. Neutron Deuteron Scattering.

So far we have been concerned only with two particle scattering processes. We shall show that the methods which we have developed can be extended to many particle collisions. In this section the simplest collision of this type, namely that

between a neutron and deuteron, will be considered. Our procedure will be modeled after method 3 in section I.2., but method 2 is equally well suited for many particle collisions.

The wave equation for the system of the two neutrons, "1" and "2", and the proton, "3", is by (0.2) and (0.5)

$$(6.1)\quad \left\{ T + V(12) + V(23) + V(31) \right\} \Psi = (E_n + E_d)\Psi$$

where T can be written as

$$(0.5)\quad T = -\frac{\hbar^2}{2M}\left(2\bar{\nabla}_{\rho_1}^2 + \frac{3}{2}\bar{\nabla}_{r_1}^2 \right)$$ [42.]

To remove the cumbersome factor in T, we make the following definitions:

$$(6.2)\quad \begin{pmatrix} D \\ U_{ij} \\ K^2 \\ \epsilon_D \end{pmatrix} = \frac{4M}{3\hbar^2} \begin{pmatrix} T \\ V(ij) \\ E_n \\ E_D \end{pmatrix}$$

---

42. For the definition of the relative coordinates, see (0.3) and (0.4).

Thus

$$D = -\left(\nabla_{r_1}^2 + \frac{4}{3}\nabla_{\rho_1}^2\right) \tag{6.3}$$

We now define

$$P \equiv -D - v_{12} - v_{23} - v_{31} + K^2 + \epsilon_0 \tag{6.4}$$

so that (6.1) can be written in the form

$$P\Psi = 0 \tag{6.5}$$

Now consider the expression

$$I_a = \int_{V_a} \Psi^* P \Psi \, (dr_1)(dr_2), \tag{6.6}$$

where V_a is the volume bounded by the five dimensional surfaces,

$$\begin{aligned} \Sigma_a^{(1)} &: r_1 = a \\ \Sigma_a^{(2)} &: r_2 = a \end{aligned} \tag{6.7}$$

Clearly

$$\delta I_a = \int_{V_a} \left\{ \Psi^*(-D)\,\delta\Psi - \delta\Psi\,(-D)\,\Psi^* \right\} (dr_1)(dr_2). \tag{6.8}$$

We aim to convert this into a surface integral over the surfaces

$\sum_a^{(1)}$ and $\sum_a^{(2)}$ and therefore express D symmetrically in terms of r_1 and r_2, namely

$$D = -\left(\nabla_{r_1}^2 - \nabla_{r_1}\cdot\nabla_{r_2} + \nabla_{r_2}^2\right) \tag{6.9}$$

as can be easily checked. Hence δI is the sum of three terms,

$$\delta I = K + L + M \tag{6.10}$$

where

$$K = \int_{V_a} \left(\Psi^* \nabla_{r_1}^2 \delta\Psi - \delta\Psi \nabla_{r_1}^2 \Psi^*\right)(dr_1)(dr_2)$$

$$L = -\int_{V_a} \left(\Psi^* \nabla_{r_1}\cdot\nabla_{r_2} \delta\Psi - \delta\Psi \nabla_{r_1}\cdot\nabla_{r_2} \Psi^*\right)(dr_1)(dr_2) \tag{6.11}$$

$$M = \int_{V_a} \left(\Psi^* \nabla_{r_2}^2 \delta\Psi - \delta\Psi \nabla_{r_2}^2 \Psi^*\right)(dr_1)(dr_2)$$

According to the exclusion principle Ψ must be antisymmetrical in the indices 1 and 2. Hence if we insist that our trial functions have the same property, then $\delta\Psi$ will also be antisymmetrical so that $M = K$. K and L can now be expressed as surface integrals by Green's theorem:

$$K = \int_{V_a} \nabla_{r_1} \left(\Psi^* \nabla_{r_1} \delta\Psi - \delta\Psi \nabla_{r_1} \Psi^* \right) (dr_1)(dr_2)$$

(6.12)

$$= \int_{v_a^{(2)}} \int_{S_a^{(1)}} \left(\Psi^* \nabla_{r_1} \delta\Psi - \delta\Psi \cdot \nabla_{r_1} \Psi^* \right) \hat{r}_1 \, ds_1 \, (dr_2)$$

where $\hat{r}_1 = r_1 / r_1$, $v_a^{(2)}$ is the three dimensional space $r_2 \leq a$ and $S_a^{(1)}$ is the two dimensional surface $r_1 = a$. Thus, the integral (6.12) extends over a portion of the five dimensional surface $\Sigma_a^{(1)}$. Similarly

$$L = \int_{V_a} \tfrac{1}{2} \nabla_{r_1} \left(\Psi^* \nabla_{r_2} \delta\Psi - \delta\Psi \nabla_{r_2} \Psi^* \right) (dr_1)(dr_2)$$

(6.13)

$$+ \int_{V_a} \tfrac{1}{2} \nabla_{r_2} \left(\Psi^* \nabla_{r_1} \delta\Psi - \delta\Psi \nabla_{r_1} \Psi^* \right) (dr_1)(dr_2)$$

$$= \int_{v_a^{(2)}} \int_{S_a^{(1)}} \left(\Psi^* \nabla_{r_2} \delta\Psi - \delta\Psi \nabla_{r_2} \Psi^* \right) \hat{r} \, ds_1 \, (dr_2)$$

since, because of the antisymmetry of Ψ , the two parts of L are equal.

We now insist that a is so large that the following two conditions are satisfied: At $r_1 \geq a$, the wave function has split into a function $\varphi(\rho_1)$ describing the deuteron, 2 and 3, and a function $F(r_1)$ describing its motion relative to the neutron 1; i.e.

(6.14) $$\Psi = \varphi(\rho_1) F(r_1) + \gamma_1 \qquad r_1 \geq a.$$

where γ represents a negligible contribution from decaying modes. And further a must be so large that

(6.15) $\varphi(\rho_1) \quad = \quad$ negligible, $\quad \rho_1 \geq \frac{2}{3} a$.

We restrict our trial functions to those which satisfy corresponding conditions, viz.

(6.14') $\Psi_* = \varphi_*(\rho_1) F_*(r_1) + \gamma_*, \quad r_1 \geq a$

and

(6.15') $\varphi_*(\rho_1) \quad = \quad$ negligible, $\quad \rho_1 \geq \frac{2}{3} a$.

We assume that both $\varphi(\rho_1)$ and $\varphi_*(\rho_1)$ are normalized. $F(r_1)$ will have different forms depending on which phase we are dealing with. We shall assume that its angular part is normalized to 4π. Thus for S - scattering,

(6.16) $$F(r_1) = A \frac{\sin kr_1}{r_1} + B \frac{\cos kr_1}{r_1}$$

$$B/A = \tan \eta$$

and similarly for higher angular momenta.

If we neglect γ and γ_*, the integrands occurring on the right hand sides of (6.12) and (6.13) are expressed most simply as functions of ρ_1 and r_1 (see (6.14) and

(6.14')) so that it is of advantage to use these coordinates as variables of integration. Therefore we transform from r_1 , r_2 to ρ_1 , ρ_2 according to the equations

(6.17)
$$r_1 = r_1$$
$$\rho_1 = \frac{2}{3} r_1 + \frac{4}{3} r_2$$

which are a consequence of the definitions (0.3) and (0.4). It follows that

(6.18) $$(dr_1)(d\rho_1) = \left(\frac{4}{3}\right)^3 (dr_1)(dr_2)$$

Also:

(6.19)
$$\nabla_{r_1})_{r_2} = \frac{2}{3} \nabla_{\rho_1})_{r_1} + \nabla_{r_1})_{\rho_1}$$
$$\nabla_{r_2})_{r_1} = \frac{4}{3} \nabla_{\rho_1})_{r_1}$$

Now for $r_1 = a$, Ψ has the form (6.14) and $\delta\Psi$ is

(6.20) $$\delta\Psi = \varphi(\rho_1)\, \delta F(r_1) + \delta\varphi(\rho_1)\, F(r_1).$$

Hence the gradient terms in (6.12) are

(6.21) $$\nabla_{r_1}\Psi = \frac{2}{3} \varphi'(\rho_1) F(r_1) \hat{\rho}_1 + \varphi(\rho_1) F'(r_1) \hat{r}_1$$

$$\nabla_{r_1}\delta\Phi = \tfrac{2}{3}\varphi'(\rho_1)\,\delta F(r_1)\,\hat{\rho}_1 + \varphi(\rho_1)\,\delta F'(r_1)\,\hat{r}_1$$

(6.22)

$$+\tfrac{2}{3}\,\delta\varphi'(\rho_1)\,F(r_1)\,\hat{\rho}_1 + \delta\varphi(\rho_1)\,F'(r_1)\,\hat{r}_1 ,$$

where $\hat{r}_1 = r_1/r_1$, $\hat{\rho}_1 = \rho_1/|\rho_1|$ and $F'(r_1)$, $\delta F'(r_1)$ denote the derivative of $F(r_1)$ and $\delta F(r_1)$ along the outward normal. Let us first integrate over the ρ_1-space, keeping r_1 fixed. The integration extends over all points with the fixed r_1 and $r_2 \le a$. Since $r_1 = a$, it follows from (6.17) that at all points outside this region $\rho_1 \ge \frac{2}{3}a$; hence, in virtue of (6.15) and (6.15'), we may extend the integral over the entire ρ_1 -space. Furthermore, since $\varphi(\rho_1)$ and $\delta\varphi(\rho_1)$ are independent of the direction of ρ_1 we can first carry out the integration over the angle between r_1 and ρ_1 , in which all terms involving $\hat{r}_1 \cdot \hat{\rho}_1$ give zero, while those involving $\hat{r}_1 \cdot \hat{r}_1$ give 4π . Hence

$$K = \left(\frac{3}{4}\right)^3 \int_{S_a^{(1)}} dS_1 \int_{|\rho_1|=0}^{\infty} 4\pi\rho_1^2\, d|\rho_1| .$$

(6.23)

$$\Big\{ \varphi^2(\rho_1)\,F^*(r_1)\,\delta F'(r_1) + \varphi(\rho_1)\,\delta\varphi(\rho_1)\,F^*(r_1)\,F'(r_1)$$

$$- \varphi^2(\rho_1)\,F^{*\prime}(r_1)\,\delta F(r_1) - \varphi(\rho_1)\,\delta\varphi(\rho_1)\,F(r_1)\,F^{*\prime}(r_1)\Big\}$$

$$= \left(\frac{3}{4}\right)^3 \int_{S_a^{(1)}} dS_1 \Big\{ F^*(a)\,\delta F'(a) - \delta F(a)\,F^{*\prime}(a)\Big\} ,$$

due to the normalization of $\varphi(\rho_1)$. Notice that $\delta\varphi(\rho_1)$ does not appear on the surface.

Let us now specialize to the case of S - scattering and assume that for $r_1 \geq a$, $F_\lambda(r_1)$ has the form

$$F_\lambda(r_1) = A \frac{\sin kr_1}{r_1} + B_\lambda \frac{\cos kr_1}{r_1} \tag{6.24}$$

where B_λ is chosen to give a smooth logarithmic derivative across $r_1 = a$. $F(r_1)$ has the form (6.16). Hence

$$\delta F(a) = \delta B \cdot \frac{\cos ka}{a}$$
$$\delta F'(a) = -\delta B \, k \frac{\sin ka}{a} \tag{6.25}$$

so that

$$K = -\left(\frac{3}{4}\right)^3 \cdot 4\pi k \, \delta B \cdot A. \tag{6.26}$$

Turning now to L we observe, by (6.19), that ∇_{r_2} acts only on functions of $|\rho_1|$ and that

$$\nabla_{r_2} \cdot (\text{function of } |\rho_1|) \propto \hat{\rho}_1. \tag{6.27}$$

Hence the integrand contains $\hat{\rho}_1 \cdot \hat{r}_1$ as factor and the integral over the angle between $\hat{\rho}_1$ and $\hat{r}_1$ vanishes.

Therefore, by (6.10) and (6.26)

(6.28) $$\delta I_q = 2K = -\frac{27}{8}\pi K A \delta B$$

so that

$$I_q + \frac{27}{8}\pi K A B_* = \frac{27}{8}\pi K A B$$

(6.29)

$$= \frac{27}{8}\pi K A^2 \tan\eta$$

is a stationary expression for $\tan\eta$.

In the derivation of (6.29) we have met some difficulties which did not exist in the two particle problem: The neglect of γ and γ' in (6.14) and (6.14') and the assumptions (6.15) and (6.15') introduce inaccuracies for any finite value of a, even if the interaction potential has a sharp cut-off (square well); this is in contrast to two particle collision, where the wave function has accurately the asymptotic form for all distances larger than the cut-off distance of the potential, and where assumptions of the type (6.15) , (6.15') do not enter.

This difficulty can be avoided by setting $a = \infty$ but then another difficulty is encountered. We have in our treatment neglected all second order terms. However, unless Ψ_* has the asymptotic form

(6.30) $$\Psi_* \to \varphi(\rho_1) F_*(r_1) \qquad \text{as } r_1 \to \infty$$

$$\searrow -\varphi(\rho_2) F_*(r_2) \qquad \text{as } r_2 \to \infty$$

where $\varphi(\rho)$ is the exact deuteron function and F_k is exactly sinusoidal with wave number K, the second order terms are appreciable over an infinite portion of the configuration space, and their integral, far from being negligible, makes I_∞ infinite. Thus suppose that our trial function tends to

$$(6.31)\qquad \Psi_k \to \{\varphi(\rho_1) + \delta\varphi(\rho_1)\} F_k(r_1), \quad \text{as } r_1 \to \infty$$

instead of (6.30), where F_k is sinusoidal. For large r_1,

$$(6.32)\qquad P \to \left(\nabla_{r_1}^2 + K^2\right) - \left(H_D - \epsilon_D\right)$$

where H_D is the deuteron Hamiltonian,

$$(6.33)\qquad H_D = -\frac{4}{3}\nabla_{\rho_1}^2 + v_{23}$$

Hence, from the region $r_1 > b$, say, in which (6.31) and (6.32) hold very nearly, I_∞ gets the contribution

$$\Delta I = \int_{r_2} \int_{r_1 = b}^{\infty} \left[\varphi(\rho_1) + \delta\varphi(\rho_1)\right] F_k^*(r_1) \cdot$$

$$(6.34)\qquad \left(-H_D + \epsilon_D\right)\left[\varphi(\rho_1) + \delta\varphi(\rho_1)\right] F_k(r_1)(dr_1)(dr_2)$$

$$= \left(\frac{3}{4}\right)^3 (\epsilon_D - \epsilon_D') \int_{r_1 = b}^{\infty} |F(r_1)|^2 (dr_1).$$

where ϵ_D' is the expectation value of H_D in the trial state $\varphi_D + \delta\varphi_D$. Clearly ΔJ although a second order term (since ϵ_D is stationary) is infinite.

We are thus faced with the following dilemma:

(1) If we use only an approximation for φ we must take a rather small a or else the effect (6.34) which is infinite for infinite a becomes important and our neglect of second order terms is unjustified. However, the finite a introduces an inaccuracy.

(2) If we take a infinite we must use the exact deuteron function in the asymptotic form of $\bar{\Psi}_f$ which may be inconvenient for practical purposes. (Such a procedure would be nearly impossible for more complicated collisions.)

The way out of this dilemma is suggested by (6.34), which shows just what the infinite contributions of the second order terms are and hence permits us to subtract them. This is done by replacing I_a, (6.6), by I_a', defined by

$$I_a' = \int_{V_a} \bar{\Psi}^* P' \bar{\Psi} \, (dr_1)(dr_2) \tag{6.35}$$

where

$$P' = P + \epsilon_D' - \epsilon_D$$

$$= \nabla_{r_1}^2 + \frac{4}{3}\nabla_{\rho_1}^2 - U_{12} - U_{23} - U_{31} + K^2 + \epsilon_D' . \tag{6.36}$$

Thus I_a' depends in two ways on the trial function:

(1) Through P whose form is determined by the asymptotic deuteron function.

(2) Through the trial - Ψ itself, when substituted in (6.35).

We shall show that

$$I'_{\alpha} + \frac{27}{8}\pi K A B_* = \frac{27}{8}\pi K A B + \Delta^2, \tag{6.37}$$

where Δ^2 is the integral of second order terms which decay exponentially in all but a finite region of the configuration space.

Let us denote

$$\int_{V_a} \varphi^* P \varphi \, (dr_1)(dr_2) \equiv I_a(\varphi)$$

$$\int_{V_a} \varphi^* P' \varphi \, (dr_1)(dr_2) \equiv I_a'(\varphi) \tag{6.38}$$

Then, by (6.36),

$$\begin{aligned} I_a'(\Psi_*) &= I_a(\Psi_*) + (\epsilon_D' - \epsilon_D)\int_{V_a} |\Psi_*|^2 (dr_1)(dr_2) \\ &= I_a(\Psi) + \delta I_a(\Psi) + I_a(\delta\Psi) \\ &\quad + \int_{V_a} (\epsilon_D' - \epsilon_D) |\Psi_*|^2 (dr_1)(dr_2) \end{aligned} \tag{6.39}$$

Now

$$I_a(\Psi) = 0 \tag{6.40}$$

and, as was shown above, without neglecting second order terms we have

$$\delta I_a(\Psi) = -\frac{2\gamma}{\delta}\pi\kappa A(\beta_* - B) + \mu_a \tag{6.41}$$

where $\lim_{a\to\infty} \mu_a = 0$

To estimate the last two terms of (6.39), we decompose V_a into

$$V_a^{(1)}: \quad r_1, r_2 \leq b < a$$

$$V_a^{(2)}: \quad r_1 \text{ or } r_2 > b \tag{6.42}$$

$$r_1, r_2 \leq a,$$

where b is so large that in $V_a^{(2)}$, $\bar{\Psi}$ and $\bar{\Psi}_*$ have their asymptotic forms

$$\bar{\Psi} = \varphi(\rho_1) F(r_1), \quad \bar{\Psi}_* = \varphi_*(\rho_1) F_*(r_1) \tag{6.43}$$

or the corresponding expressions with 1 replaced by 2. Clearly the last two terms in (6.39) are both of the second order, so that their integral over the limited $V_a^{(1)}$ is of the type Δ^2. On the other hand in $V_a^{(2)}$ we shall find that the last two terms, give zero owing to the integration over ρ_1 (or ρ_2). Thus in the region of $V_a^{(2)}$ where $r_1 > b$, they give

$$\int \left\{ \delta\Psi^{*} P \delta\Psi + (\epsilon_D' - \epsilon_D) |\Psi_*|^2 \right\} (d\rho_1)$$

$$= \int \left\{ (\Psi_*^{*} - \Psi^{*}) P (\Psi_* - \Psi) + (\epsilon_D' - \epsilon_D) |\Psi_* - \Psi|^2 \right\} (d\rho_1)$$

(6.44) $$= \int \{ (\varphi_* F_*^{*} - \varphi F^{*}) (\nabla_{r_1}^2 + K^2 + \epsilon_D - H_D) (\varphi_* F_* - \varphi F)$$

$$+ (\epsilon_D' - \epsilon_D) \varphi_*^2 |F_* - F|^2 \} (d\rho_1)$$

$$= |F_*|^2 \int \varphi_* (-H_D + \epsilon_D') \varphi_* (d\rho_1)$$

$$= 0$$

Hence

(6.45) $$I_0(\delta\Psi) + \int (\epsilon_D' - \epsilon_D) |\Psi_*|^2 = \Delta^2$$

From (6.39), (6.40), (6.41), (6.45) we now find

$$I'_\infty(\Psi_*) = -\frac{27}{8} \pi K (B_* - B) + \Delta^2$$

which is the statement (6.37).

This means that $\tan\eta$ as calculated from

(6.46) $$I'_\infty + \frac{27}{8} \pi K A B_* = \frac{27}{8} \pi K A^2 \tan\eta$$

is stationary if we admit only such trial functions whose asymptotic form is

(6.47) $$\Psi_* \longrightarrow \varphi_*(\rho_1) \left\{ A \frac{\sin K r_1}{r_1} + B_* \frac{\cos K r_1}{r_1} \right\}$$

Thus the exact form of the internal wave function and the binding energy of the colliding nuclei are not required.

Numerical Calculations.

We have made exploratory calculations on n-d scattering in preparation for a more extensive investigation. For simplicity we have so far only used trial functions of group structure, but we remark again that this limitation is by no means inherent in our method.

We have assumed an ordinary Wigner potential

$$V_{ij} = -V_0 e^{-\frac{(r_{ij})^2}{a^2}} \tag{6.48}$$

with $V_0 = -72.00\ mc^2$ and $a = 0.8$ in units of $\lambda_0 = 2.80 \times 10^{-13}$ cm.[43] These constants give the correct binding energy of 2.18 MEV. for the deuteron.

As trial functions for S-scattering we have used

$$\Psi_u = \varphi_*(\rho_1) F_u(r_1) \chi_1 + \varphi_*(\rho_2) F_u(r_2) \chi_2 , \tag{6.49}$$

where we have set

$$\varphi_*(\rho_1) = 0.42377\, e^{-0.5\rho_1^2}$$

$$F_u(r) = c_0 + c_2 r^2 + \cdots c_{2n} r^{2n} , \quad r \le a \quad (n = 0, 1, 2) \tag{6.50}$$

(cont'd)

43. These constants are almost identical with those of Motz and Schwinger, ref.23, who however used an exchange potential.

(6.50 cont'd)

$$\chi_1 = -\chi_2 = \alpha(1)\,\alpha(2)\,\alpha(3) \qquad \text{Quartet scattering}$$

$$\left.\begin{aligned} \chi_1 &= 6^{-1/2}\big[\alpha(1)\,\alpha(2)\,\beta(3) + \\ &\quad \alpha(1)\,\beta(2)\,\alpha(3) - 2\,\beta(1)\,\alpha(2)\,\alpha(3)\big] \\ \chi_2 &= -P_{12}\,\chi_1 \end{aligned}\right\} \quad \text{Doublet scattering}$$

All distances are measured in units of r_0. $\varphi_\pi(\rho_1)$ is the best approximation of its type for the deuteron function.

The polynomial approximation for $F(r)$ has the wrong asymptotic form. Hence it was assumed to hold only inside the region $r < a$.

We have calculated only S-scattering at zero energy. Hence, asymptotically

$$(6.50') \qquad F(r) \longrightarrow A' + \frac{B'}{r}$$

where A' and B' are chosen so that the polynomial form of $F_n(r)$ passes smoothly into (6.50') at $r = a$.

As we are limiting ourselves to a finite region, the difference between I(a) and I'(a) is negligible (see (6.35) and (6.36)). The calculations to be described were carried out by using I'(a) throughout.

We have calculated $\lim_{\kappa \to 0} (\tan \eta / \kappa) = X$, for quartet and doublet scattering, which determine the total cross section in the limit of zero energy by the equation

$$(6.53) \qquad \sigma = 4\pi\left(\frac{2}{3}X_q^2 + \frac{1}{3}X_d^2\right)$$

where q and d refer to quartet and doublet scattering respectively.

In the case of doublet scattering, the convergence with increasing values of ν was slow. Since in the case of two particle scattering method 2 gave somewhat better results than method 3, (see Table I, p. 30) we have calculated X_d not only by (6.29) but also by the equation

$$(6.51) \qquad I_a + \frac{2\eta}{8}\pi a^2\left(LF^2(a) - F(a)F'(a)\right) = 0$$

which bears the same relation to (6.29) as does (2.32) to (2.23). X is determined from the logarithmic derivative L according to the equation

$$(6.52) \qquad X = -\frac{a^2 L}{aL+1}.$$

However, the convergence was only slightly improved.

The approximate values of X, obtained by our variational methods depend both on a and n. For large enough n we expect the following variation with a:

(A1) When a is too small the expression (6.29) for tan is incorrect. Hence X should depend strongly on a.

(A2) When a is sufficiently large for (6.29) to hold, X should be fairly independent of a until

(A3) a becomes so large that F_n can no longer approximate the true function over the entire interval. Our variational principle than breaks down because second order terms become important. Here again we expect a considerable variation of X with a.

Thus we expect to find an extremum in the region (A2) and the value of X at that extremum may be taken as our approximation for X.

As we increase n we expect

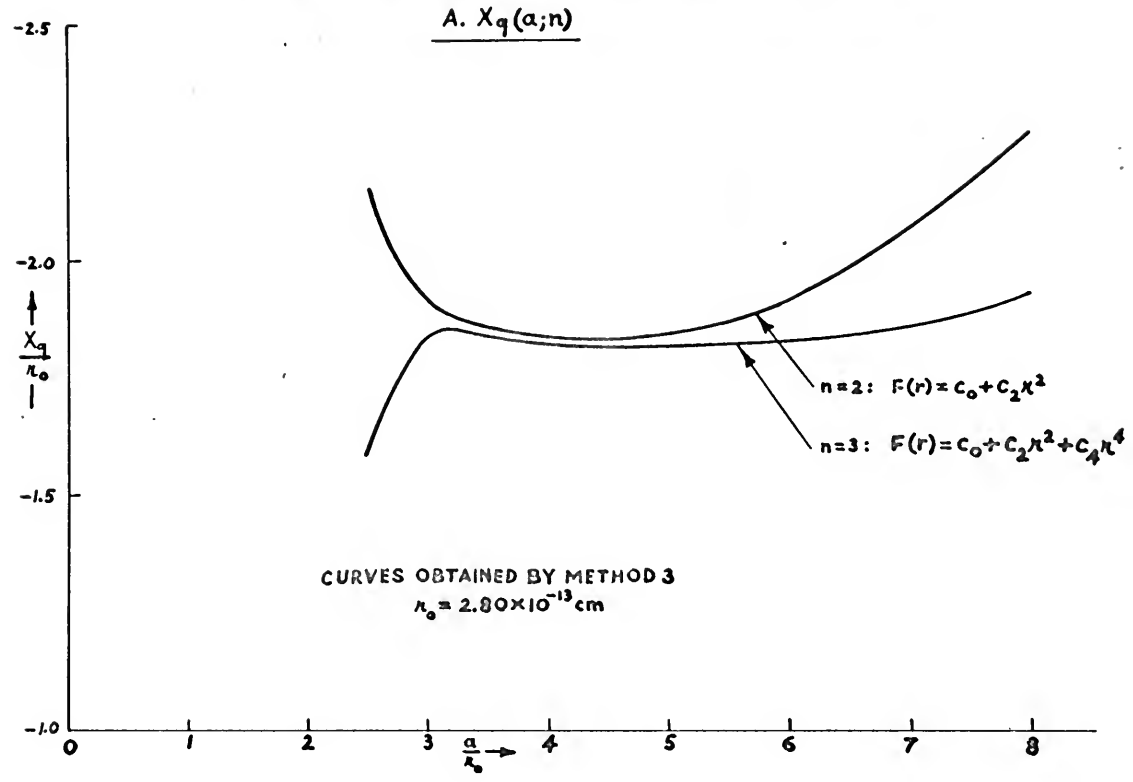
(B1) Gradual extension of the "plateau" (A2) towards larger values of a.

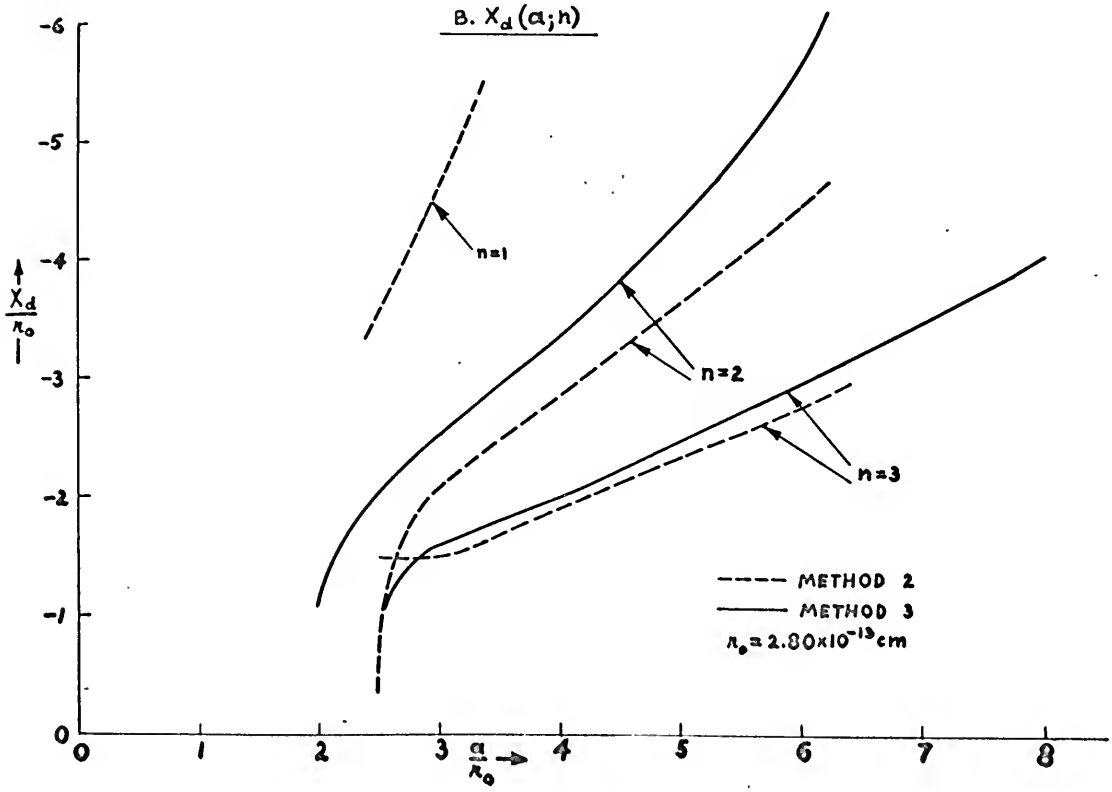
(B2) Increasingly smaller differences X (a; n + 1) - X (a; n) for large enough, fixed, a.

In an approximation method n should be increased until (B1) and (B2) are so well satisfied that further increase of n is not likely to change X appreciably.

In virtue of the choice of our potential and trial function, all integrals occurring in I_a could be analytically evaluated. Our results for X_q and $X_{\hat{d}}$ are given in Tables III, IVa and IVb and plotted in Graph 2. The best 3 - parameter wave functions, $F_2(r)$, determined in the usual way from our variational principles are shown in Graph 3.

GRAPH 2. NEUTRON DEUTERON SCATTERING





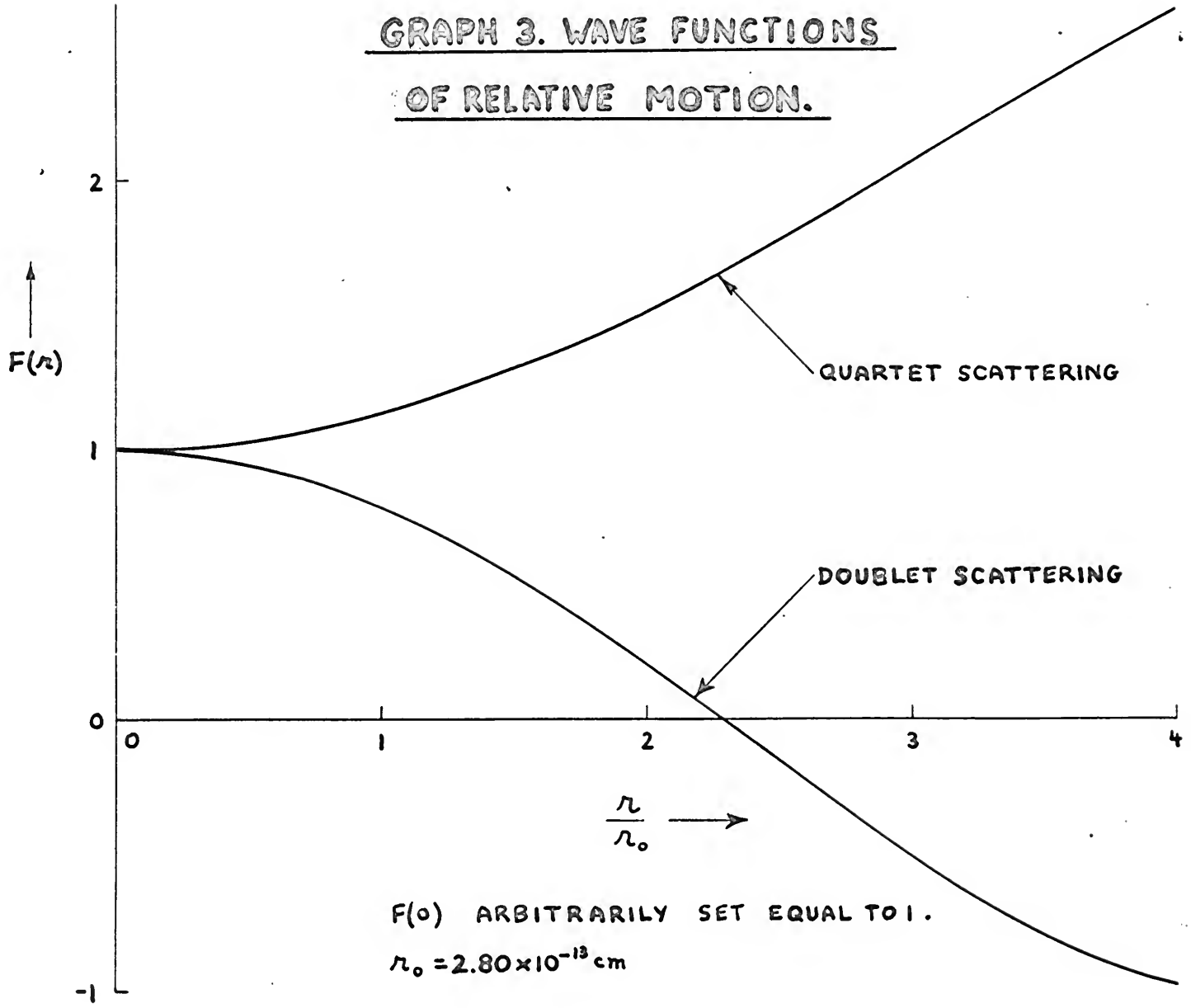

GRAPH 3. WAVE FUNCTIONS
OF RELATIVE MOTION.
2
1
0
-1
F(r)
QUARTET SCATTERING
DOUBLET SCATTERING
0
1
2
3
4
r / r₀
F(0) ARBITRARILY SET EQUAL TO 1.
r₀ = 2.80 × 10⁻¹³ cm

Table III.

Quartet Scattering : $X_q(a;n)/r_0$.

(Method 3, (6.29))

a/r_0 \ n	0	1	2
2.5	- 4.39	- 2.16	- 1.58
3.0	- 4.39	- 1.91	- 1.85
4.0	- 4.39	- 1.84	- 1.83
6.0	- 4.39	- 2.03	- 1.84
8.0	- 4.39	- 2.26	- 1.92

Table IV a.

Doublet Scattering : $X_d(a;n)/r_0$.

(Method 3, (6.29))

a/r_0 \ n	0	1	2
2.0	+ 8.53	- 1.18	- 1.58
2.5	+ 8.53	- 2.03	- 3.73
2.6	+ 8.53	- 2.14	- 1.03
3.0	+ 8.53	- 2.51	- 1.58
4.0	+ 8.53	- 3.38	- 2.01
6.0	+ 8.53	- 5.65	- 2.98
8.0	+ 8.53	- 9.16	- 4.05

Table IV b.

Doublet Scattering : X_d (a;n) / r_0.

(Method 2, (6.51), (6.52))

a/r_0 \ n	0	1	2
2.5	- 3.53	- 0.36	- 1.51
3.0	- 4.62	- 2.04	- 1.47
4.0	- 7.53	- 2.85	- 1.90
6.0	- 20.23	- 4.47	- 2.78

Interpretation of the numerical results:

A. The convergence of X_q is much more rapid than that of X_d. This is due to the fact that F(r) is more irregular for doublet scattering (see Graph 3) and therefore requires more terms for adequate approximation.

B. The variation of X_q with a and n is as expected (pp. 73 and 74); X_{ol} seems to behave in a similar manner although the number of parameters is not large enough to exhibit a proper plateau.

C. To determine the total cross section we must select the best values of X_q and X_d from our tables. In the case of X_q (Table III) we have evidently come very close to the limit which can be reached with group structure form. We see that our results depend markedly on a for values smaller than 3.

This indicates that the interaction is appreciable out to about that distance. We therefore choose $X_q = X_q(4;2) \simeq -1.83\lambda_0$. The choice of X_d is more difficult. At a = 3 we cannot be sure that the interaction is completely negligible; on the other hand at a = 4 we are still quite far from convergence. Let us nevertheless choose $X_d = X_d(4;2) \simeq -1.90\lambda_0$ (see Table IV b). This gives, by (6.53), $\sigma \simeq 3.39$ barns. If we estimate the limit of X_d which could be reached by taking larger n, as $X_d \simeq -1.50\lambda_0$, we obtain $\sigma \simeq 2.94$ barns. These figures are in qualitative agreement with the experimental value of 3.2 barns [27].

Let us summarize the possible inadequacies of this tentative calculation.

(a) Wigner forces may not be adequate to describe this process.

(b) Our approximation for $\varphi(\rho_1)$ (see (6.50)) may not be sufficiently accurate.

(c) The group structure approximation may not be adequate.

(d) The Schroedinger theory may not be capable of an accurate description of this process.

Of these shortcomings (a), (b) and (c) can be remedied by more extensive calculation of the same kind. When this is done, it will be possible to decide to what extent (d) is true.

In future calculations the following points should be given consideration:

(1) Terms allowing for the polarization of the deuteron

should be introduced.

(2) It may be of advantage to use trial - F's of the correct asymptotic form. The reason for this is the following: If we use a polynomial expression for F (r), we must include a large number of terms since, due to the loose structure of the deuteron, the region of interaction is very large ($\approx$ 8×10^{-13} cm). This necessitates the calculation of a great many matrix elements, which is probably more laborious than the numerical integrations which become necessary when functions of the correct asymptotic form are used.

I.7. The General Case of Composite Collisions.

The method used in the preceeding section can be extended to all collisions of composite nuclei in which triple or multiple disintegrations are energetically forbidden. The analytic aspects of the problem are quite analogous to those encountered in n-d scattering. However the combinatorial side of the general problem is somewhat complicated and no detailed description of the general case will be given here. We shall merely mention a few points of interest.

Modes of Collision.

Our picture is the following: We have a number of pairs of nuclei colliding and a number of pairs (possibly different ones) emergin after the collision. The groupings of nucleons

into pairs are alternative (not independent) processes, each pair comprising the same nucleons. There is, then a "region of interaction" in the configuration space, where all nucleons are close together, and an "asymptotic region", where the nucleons have separated into pairs.

On a hyper-surface, Σ , separating the two regions, the wave function has the form

$$(7.1)\quad \Psi = \sum \Phi_i$$

where, if $\varphi_i^{(1)}$ and $\varphi_i^{(2)}$ describe the normalized internal wave functions of two colliding nuclei and F their relative motion,

$$(7.2)\quad \Phi_i = \varphi_i^{(1)} \varphi_i^{(2)} F_i .$$

A function of the type (7.2) will be called a mode of collision.

If Ψ is a proper function of a complete set of operators (H, J, P, J_z..), its modes satisfy the following asymptotic orthogonality conditions:

$$(7.3)\quad \int_\Sigma \Phi_i \Phi_j^* \, d\sigma = 0 \quad , \; i \neq j .$$

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44. The term "collide" will be used in the remainder of this section to describe both collisions and disintegrations.

For if Φ_i and Φ_j describe different pairs of nuclei, they exist on different portions of the hypersurface Σ and hence (7.3) is satisfied. If however they describe the same pair of nuclei, then either $\varphi_i^{(1)} \neq \varphi_j^{(1)}$ or $\varphi_i^{(2)} \neq \varphi_j^{(2)}$, so that the orthogonality (7.3) follows from the integration over the internal coordinates of the nuclei.

Number of Arbitrary Constants of the Scattering Matrix.

We have remarked in section I.5. that due to its unitary character and symmetry, the two dimensional scattering matrix involves only three independent constants. In the present case the scattering matrix has the same order, n, as there are different modes of collision. When represented in the scheme of incoming and outgoing modes, we have proved that the number of independent constants is $\frac{(n)\ (n+1)}{2}$. Only this many constants need to be determined.

Rayleigh-Ritz Method.

We have already applied the Rayleigh-Ritz method to two problems involving two modes of collision: n-p scattering with tensor forces (section I.5.) and n-d scattering (section I.6.). In section I.5. we have discussed two different variational methods: One dealing with complex (running) wave functions and yielding all elements of the scattering matrix; the other dealing with standing waves and giving only the proper values of the scattering matrix. (Only this second method was used in n-d scattering.)

These methods can be generalized as follows:

Running waves:

When dealing with a special case of running waves in section I.5., we introduced a wave function, Ψ_1, (5.5), whose angular and spin functions were the complex conjugates of those of the function Ψ_2. This was done in order to make use of the orthogonality relation, corresponding to (7.3)

In the present more general case, such a procedure is not convenient, since the wave function does not everywhere separate into radial and angular parts. On the other hand, if we take the complex conjugate of the entire function, the sense of the incoming and outgoing waves is reversed and the α's and β's, denoting their amplitudes are mixed up. To avoid this difficulty we use the following notation:

$$\Psi^{(-\mu)} = \Psi^{(\mu)*} \tag{7.4}$$

where $\Psi^{(\mu)}$ and $\Psi^{(-\mu)}$ have the asymptotic forms

$$\left.\begin{aligned} \Psi^{(\mu)} &= \sum_i \varphi_i^{(1)} \varphi_i^{(2)} \left(\alpha_i^{(\mu)} \frac{e^{-iK_i r_i}}{r_i} + \beta_i^{(\mu)} \frac{e^{iK_i r_i}}{r_i} \right) \cdot S_i \\ \Psi^{(-\mu)} &= \sum_i \varphi_i^{(1)*} \varphi_i^{(2)*} \left(\alpha_i^{(-\mu)} \frac{e^{-iK_i r_i}}{r_i} + \beta_i^{(-\mu)} \frac{e^{iK_i r_i}}{r_i} \right) \cdot S_i^* \end{aligned}\right\} \text{ on } \Sigma. \tag{7.5}$$

S_i is the angular function of relative motion of the mode Φ_i. We note that by the definition (7.4),

$$\alpha_i^{(-\mu)} = \beta_i^{(\mu)*} \; ; \; \beta_i^{(-\mu)} = \alpha_i^{(\mu)*}, \tag{7.6}$$

which is the reason for introducing $\Psi^{(-\mu)}$, as only in this way can the α's and β's remain associated with incoming and outgoing waves respectively.

We now form the expression

$$(7.7)\quad I_{21} = \int_V \bar{\Psi}^{(-1)} \left(-H + E\right) \bar{\Psi}^{(2)}\, d\tau$$

where $\bar{\Psi}^{(1)}$ and $\bar{\Psi}^{(2)}$ have the same quantum numbers, V is the region of interaction, H the total Hamiltonian and E the total energy of the system. The first variation of I_{21} can be transformed into a surface integral in the usual way and we are led to

$$(7.8)\quad \begin{aligned} \delta I_{21} &= \int_\Sigma \left\{ \bar{\Psi}^{(-1)} \frac{\partial}{\partial n} \delta \bar{\Psi}^{(2)} - \delta \bar{\Psi}^{(2)} \frac{\partial}{\partial n} \bar{\Psi}^{(-1)} \right\} d\sigma \\ &= \sum \hbar^2_i \bar{K}_i \alpha_i^{(-1)} \delta \beta_i^{(2)} \qquad \left(\begin{array}{l} \bar{K}_i = K_i / M_i \\ M_i = \text{red. mass} \end{array} \right) \end{aligned}$$

(Compare (5.7)) Therefore the following equation is stationary relative to variations of $\bar{\Psi}^{(1)}$ and $\bar{\Psi}^{(2)}$.

$$(7.9)\quad I_{21} + \frac{\hbar^2}{i} \sum_i \bar{K}_i \alpha_i^{(-1)} \beta_{i,\text{trial}}^{(2)} = \frac{\hbar^2}{i} \sum_i K_i \alpha_i^{(-1)} \beta_i^{(2)}.$$

We would like to convert this into a stationary expression for the elements of the scattering matrix (see (5.9)). Now in the case where groups may collide with different kinetic energies, we must modify the

definition of the scattering matrix given in (5.1). The amplitudes β_i are linear combinations of the α_i, viz.

$$\beta_i = \sum_j c_{ij} \alpha_j . \tag{7.10}$$

The total flux into the region of the configuration space enclosed by Σ is

$$\begin{aligned} 0 &= \sum_i \bar{K}_i \left\{ |\alpha_i|^2 - |\beta_i|^2 \right\} \\ &= \sum_i \left\{ \bar{K}_i |\alpha_i|^2 - \bar{K}_i \sum_j |c_{ij}|^2 |\alpha_j|^2 \right\} \qquad (7.11) \\ &= \sum_i \left\{ \left| \sqrt{\bar{K}_i}\, \alpha_i \right|^2 - \sum_j \left| \sqrt{\frac{\bar{K}_i}{\bar{K}_j}}\, c_{ij} \right|^2 \left| \sqrt{\bar{K}_j}\, \alpha_j \right|^2 \right\} \end{aligned}$$

The last line shows [46] that the matrix

$$S = \left(\sqrt{\frac{\bar{K}_i}{\bar{K}_j}}\, c_{ij} \right) \tag{7.12}$$

is unitary, and hence may properly be taken to be the scattering matrix. If in analogy with (5.2) we define

$$A = \begin{pmatrix} \sqrt{\bar{K}_1}\, \alpha_1 \\ \sqrt{\bar{K}_2}\, \alpha_2 \\ \vdots \end{pmatrix}, \qquad B = \begin{pmatrix} \sqrt{\bar{K}_1}\, \beta_1 \\ \sqrt{\bar{K}_2}\, \beta_2 \\ \vdots \end{pmatrix} \tag{7.13}$$

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46. A. Wintner, Spektraltheorie der Unendlichen Matrizen, (Leipzig, 1929) p. 34.

then by (7.10) and (7.12),

$$B = S \cdot A. \tag{7.14}$$

In this notation (7.9) can be written as

$$I_{21} + \frac{\hbar^2}{i} A^{(1)} \cdot B^{(2)}_{trial} = \frac{\hbar^2}{i} A^{(1)} \cdot S \cdot A^{(2)} \tag{7.15}$$

Hence by choosing our trial functions with only a single non-vanishing component of A, we can obtain a stationary expression for any one matrix element of S at a time.

Standing Waves:

The modes of the proper functions of the scattering matrix all have the same phase shift (see section I.5., (5.15) ff.) We form

$$I = \int_V \Psi^* (-H + E) \bar{\Psi} \, d\tau \tag{7.16}$$

where $\bar{\Psi}$ is a trial function which consists, asymptotically, of standing waves. The first variation of I now becomes

$$\delta I = -\frac{\hbar^2}{2} \sum \bar{K}_i A_i^2 \, \delta \tan \eta_i, \tag{7.17}$$

where A_i is the amplitude of $\sin K_i r_i / r_i$ in F, the function of relative motion.

Hence

$$I + \sum \frac{h^2}{2} \bar{K}_i A_i^2 \tan \eta_i, \text{ trial}$$

(7.18)

$$= \sum \frac{h^2}{2} \bar{K}_i A_i^2 \tan \eta .$$

The collision determinant, which arises on application of the Rayleigh-Ritz method is of the n^{th} degree corresponding to the sum of n squares multiplying tan η. Its n solutions are approximations for the tangents of the n proper values of the phase shift.

II. THE VARIATION ITERATION METHOD IN COMPOSITE COLLISIONS.

II.8. Preliminary Considerations.

Schwinger[41] has recently developed a variation iteration method for two particle collisions. His treatment leads to a stationary expression for $\tan\eta$, involving a Green's function and giving very good results, even with rather crude trial functions. In this section we shall first rederive his results in a slightly different way, to show its relation to the bilinear variational principles discussed in Part I; and then shall examine this method with a view of generalizing it to many particle problems.

Consider first the one dimensional Schroedinger equation,

$$(8.1)\quad \left[\frac{d^2}{dx^2} + K^2 + \lambda f(x)\right] u(x) = 0,$$

where u satisfies the boundary conditions

$$(8.2)\quad u(0) = 0\ ;\ u(x) \longrightarrow \sin Kx + \tan\eta \cdot \cos Kx \quad \text{as } x \to \infty.$$

Let the Green's function $G(x, x')$ satisfy the differential equation

$$(8.3)\quad \left(\frac{d^2}{dx^2} + K^2\right) G(x, x') = -\delta(x - x'),$$

and certain boundary conditions to be determined later. Multiplying (8.1) by G and (8.3) by u, and integrating over x from 0 to a we find

$$G(x,x')\frac{d}{dx}u(x) - u(x)\frac{d}{dx}G(x,x')\Big|_0^a$$

$$+\lambda\int_0^a G(x,x')\,f(x)\,u(x)\,dx = u(x') \tag{8.4}$$

To make the integrated terms vanish we now impose the same boundary conditions on G as are satisfied by u, namely

$$G(0,x') = 0$$

$$G(x,x') \longrightarrow F(x')(\sin Kx + \tan\eta\cdot\cos Kx), \text{ as } x\to\infty, \tag{8.5}$$

where F (x') is some function of x'. The solution of (8.3) and (8.5) is

$$G(x,x') = \frac{1}{K}\sin Kx_<\cdot\cos Kx_> + \frac{\cot\eta}{K}\sin Kx\cdot\sin Kx' \tag{8.6}$$

In virtue of (8.4) and (8.5) we now obtain, on letting $a\to\infty$,

$$u(x) = \lambda\int_0^\infty G(x,x')\,f(x')\,u(x')\,dx'. \tag{8.7}$$

This may be regarded as a proper value problem for λ, for a given $\cot\eta$, and the discussion can be completed from this point of view: (8.7) is multiplied by f(x)u(x) and

integrated over x, giving

$$\int_0^\infty f(x)\left[u(x)\right]^2 dx = \lambda \frac{\cot\eta}{K}\left[\int_0^\infty \sin Kx \cdot f(x)\, u(x)\, dx\right]^2$$

(8.8)

$$+\lambda\int_0^\infty f(x)\, u(x)\, G_0(x,x')\, f(x')\, u(x')\, dx\, dx'$$

where

(8.9) $$G_0(x,x') = \frac{1}{K}\sin K x_< \cdot \cos K x_>.$$

(8.7) is a stationary expression for λ corresponding to a given $\cot\eta$ or for $\cot\eta$ corresponding to a given λ.

On the other hand we may derive (8.8) as follows: We note that u_2 defined by

(8.10) $$u_2 = \lambda\int_0^\infty G(x,x')\, f(x')\, u(x')\, dx',$$

becomes, asymptotically

$$u_2 \longrightarrow (\sin Kx + \tan\eta \cdot \cos Kx).$$

(8.11)

$$\frac{\lambda\cot\eta}{K}\int_0^\infty \sin Kx'\, f(x')\, u(x')\, dx'$$

and thus has the correct asymptotic form and phase shift for <u>any</u> trial u; furthermore by (8.7), $u_2 = u$ when u is the correct solution. Hence if used in our bilinear

variational principle (2.48), in conjunction with $u_1 = u$, we have simply

$$I_{21} = \int_0^\infty \left\{ u \left[\frac{d^2}{dx^2} + K^2 + \lambda f(x) \right] \right.$$

$$(8.12)\quad \left. \lambda \int_0^\infty \left(G_0(x,x') + \frac{\cot \eta}{K} \sin Kx \cdot \sin Kx' \right) f(x') u(x') dx' \right\} dx$$

$$= 0 ;$$

$$\delta I_{21} = 0$$

for arbitrary variations of u. This is of course equivalent to (8.8).

Three Dimensional Formulation.

Turning now to the solution of the equation

$$(8.13)\quad \left[\nabla^2 + K^2 + \lambda f(r) \right] \psi(r) = 0.$$

one can proceed in an entirely analogous manner. The solution of (8.13) corresponding to a wave of unit amplitude incident along K_2 is written in the form

$$(8.14)\quad \psi_{K_2} = e^{iK_2 \cdot r} + \lambda \int \frac{e^{iK|r-r'|}}{4\pi |r-r'|} f(r') \psi_{K_2}(r') (dr')$$

and becomes asymptotically

$$(8.15)\quad \psi_{K_2} \longrightarrow e^{iK_2 \cdot r} + \frac{e^{iKr}}{r} \frac{\lambda}{4\pi} \int e^{-iK \cdot r'} f(r') \psi_{K_2}(r') (dr')$$

Hence the scattering amplitude in the direction K_1 is

given by

$$f(K_2, K_1) = \frac{\lambda}{4\pi} \int e^{-iK_1 \cdot r'} f(r') \psi_{K_2}(r') (dr'). \tag{8.16}$$

This permits us to write (8.14) in the homogeneous form

$$\psi_{K_2}(r) = \lambda \int G(r, r') f(r') \psi_{K_2}(r') (dr') \tag{8.17}$$

where

$$G(r, r') = \frac{1}{4\pi f(K_2, K_1)} e^{iK_2 \cdot r} \cdot e^{-iK_1 \cdot r'} + \frac{e^{ik|r-r'|}}{4\pi |r-r'|} \tag{8.18}$$

For large values of r, (8.17) becomes, in the direction K_1,

$$\psi_{K_2}(r) \longrightarrow \frac{\lambda}{4\pi f(K_2, K_1)} \left(e^{iK_2 \cdot r} + f(K_2, K_1) \frac{e^{ikr}}{r} \right) \int e^{-iK_1 \cdot r'} f(r') \psi_{K_2}(r') (dr'). \tag{8.19}$$

Hence no matter what function $\psi_{K_2}(r')$ is substituted in the right hand side of (8.17), the left hand side always has the correct scattering amplitude $f(K_2, K_1)$. This, in fact, is the reason for replacing (8.14) by (8.17).

Returning to the variational principle (4.10), it is clear that if we use only such ψ_{K_2} which have the form

$$\psi_{K_2}(r) = \lambda \int G(r, r') f(r') \varphi_{K_2}(r') (dr'), \tag{8.20}$$

and arbitrary $\psi_{K_1}(r)$, then since $f^{(2)}_{\pm}(K_2, K_1) = f(K_2, K_1)$ it reduces to $I_{K_2 K_1} = 0$. When this is written out in full, it serves as a variational principle for the determination of $f(K_2, K_1)$:

$$\frac{\lambda}{4\pi f(K_2,K_1)} \int \psi_{-K_1}(r) f(r) e^{iK_2 \cdot r} (dr) \cdot \int \varphi_{K_2}(r') f(r') e^{-iK_1 \cdot r'} (dr')$$

$$(8.21) \quad - \int \psi_{-K_1}(r) f(r) \varphi_{K_2}(r) (dr) \cdot$$

$$+ \lambda \int \psi_{-K_1}(r) f(r) \frac{e^{iK|r-r'|}}{4\pi |r-r'|} \varphi_{K_2}(r') f(r') (dr) (dr') = 0$$

Let us note specially that no boundary conditions had to be imposed on either ψ_{-K_1} or φ_{K_2}. This is in keeping with the fact that all integrals occuring in (8.21) extend only over the region of interaction, where f(r) and f(r') are not zero.

The one and three dimensional treatments have in common certain features which may be expected to carry over into a similar treatment of composite scattering processes:

A. Both treatments involve one iteration ((8.10) and (8.20)) and hence give excellent results even with poor trial functions. In principle the accuracy can be increased by iterating a number of times.

B. The trial functions need not satisfy any boundary conditions; instead,

C. The boundary conditions are automatically satisfied by a proper choice of the Green's function.

D. The Green's function

1. except for the inhomogeneous term, satisfies the same differential equation as does the wave function asymptotically (see (8.3) and (8.18)) and

2. has the same phase shift (or scattering amplitude) as the correct wave function.

II.9. Neutron Deuteron Scattering: Six Dimensional Green's Functions.

As a prototype of composite scattering processes we shall consider in this section the collision of a neutron with a deuteron. We shall generalize the method described in the last section in a straightforward manner, but shall find that for composite scattering it is too complicated to be of practical use.

The wave equation for our system is, by (6.3) - (6.5)

$$(9.1)\qquad P\Psi \equiv \left(-D - U_{12} - U_{23} - U_{31} + K^2 + \epsilon_D\right)\Psi = 0,$$

where

$$(9.2)\qquad D = -\left(\nabla_{r_1}^2 + \frac{4}{3}\nabla_{\rho_1}^2\right) = -\left(\nabla_{r_2}^2 + \frac{4}{3}\nabla_{\rho_2}^2\right).$$

Let us for the moment ignore the spin dependence and simply insist that the wave function be antisymmetrical in 1 and 2. Then, asymptotically the S-wave has the form:

$$(9.3)\qquad r_1 \to \infty : \Psi \to \varphi(\rho_1)\ \frac{\sin Kr_1 + \tan\eta \cdot \cos Kr_1}{r_1}$$

$$r_2 \to \infty : \Psi \to -\varphi(\rho_2)\ \frac{\sin Kr_2 + \tan\eta \cdot \cos Kr_2}{r_2}$$

The wave equation (9.1) becomes asymptotically:

$$(9.4)\qquad r_1 \to \infty : L_1\Psi = 0 \to \left[\left(\nabla_{r_1}^2 + K^2\right) + \left(\frac{4}{3}\nabla_{\rho_1}^2 - v_{23} + \epsilon_D\right)\right]\Psi = 0.$$

$$r_2 \to \infty : L_2\Psi = 0 \to \left[\left(\nabla_{r_2}^2 + K^2\right) + \left(\frac{4}{3}\nabla_{\rho_2}^2 - v_{13} + \epsilon_D\right)\right]\Psi = 0.$$

According to D.1., section II.8, the Green's function should satisfy the differential equation

$$(9.5)\qquad L\,G = -\delta(r_1 - r_1')\,\delta(r_2 - r_2')$$

in the asymptotic region of the configuration space, where L reduces to L_1 and L_2 for large values of r_1 and r_2 respectively. In the one dimensional problem L was simply $\frac{d^2}{dx^2} + K^2$ and made no reference to the interaction potential; hence a solution for G could be easily found.

The fundemental difficulty in the case of composite collisions is that parts of the interaction, namely the internal forces of the colliding nuclei, persist at infinity. Therefore they appear in the asymptotic operators L and L and hence also in L, which makes the determination of G practically impossible. In fact the simplest L which we can choose is $L = P + v_{12}$, since v_{12} is the only interaction which disappears asymptotically. Of course the practical solution of

$$(9.6) \qquad \left(-D - v_{23} - v_{31} + k^2 + \epsilon_D\right) G = -\delta(r_1 - r_1')\,\delta(r_2 - r_2')$$

is quite impossible.

For this reason we shall not pursue this method any further, but merely state that if formally carried through, it has the properties A, B, C and D mentioned in the last section and leads to stationary expressions for the elements

$$(9.7) \qquad f\left(K_\alpha^{(i)}, K_\beta^{(j)}\right) \qquad i = 1,2\ ;\ j = 1,2$$

of the scattering matrix (i and j refer to the incoming and outgoing neutrons, K_α and K_β to their directions).

Another formulation which suggests itself is analogous to the treatment of the bound state: We write the wave equation as

$$(9.8) \qquad \left(\nabla_{r_3}^2 + \frac{4}{3}\nabla_{\rho_3}^2 + k^2 + \epsilon_D\right)\Psi = \left(v_{12} + v_{23} + v_{31}\right)\Psi$$

and introduce a Green's function to satisfy

$$(9.9)\quad \left(\nabla_{r_3}^2 + \tfrac{4}{3}\nabla_{\rho_3}^2\right) G(r_3, \rho_3 ; r_3', \rho_3') = -\delta(r_3 - r_3')\,\delta(\rho_3 - \rho_3').$$

A solution of this equation is

$$(9.10)\quad G = \frac{1}{3^{1/2}\,4\pi^4}\,\frac{1}{r}\frac{\partial}{\partial r}\,\frac{1}{\rho}\frac{\partial}{\partial \rho}\,H_0\left(i(k^2+\epsilon_D)\sqrt{\tfrac{2}{3}r^2+\tfrac{1}{2}\rho^2}\right)$$

where

$$(9.11)\quad r = |r_3 - r_3'|,\qquad \rho = |\rho_3 - \rho_3'|.$$

Since $k^2+\epsilon_D$ is negative in our case, G falls off exponentially. Hence, on multiplying (9.8) by G, (9.9) by Ψ, subtracting and integrating over r_3 and ρ_3, the surface integral vanishes and we are left with

$$(9.12)\quad \Psi(r_3', \rho_3') = \int G(r_3', \rho_3' ; r_3, \rho_3)\left(v_{12}+v_{23}+v_{31}\right)\Psi(r_3\rho_3)\,(dr_3)(d\rho_3)$$

However the exponential vanishing of G wipes out all reference to the boundary, from where in the past we had always derived the connection with the scattering properties. Thus the present formulation, while providing an iteration procedure for the collision wave function, does not lead to a stationary expression for the phase shift or scattering amplitude.

II.10. Neutron Deuteron Scattering: Three Dimensional Green's Function.

Since, as we have seen, the straightforward generalization of the two particle procedure is of no practical use we have tried the following alternative approach:

Where $r_1 \to \infty$, the wave function separates and therefore satisfies not only $L_1 \Psi = 0$ (see (9.4)) but also

$$(10.1) \qquad r_1 \longrightarrow \infty : \left(\nabla_{r_1}^2 + K^2\right) \Psi(\rho_1, r_1) = 0$$

Hence, in partial agreement with D.2 (section II.1.) we introduce a three dimensional Green's function, which satisfies

$$(10.2) \qquad \left(\nabla_{r_1}^2 + K^2\right) G(r_1, r_1') = -\delta(r_1 - r_1')$$

and has the correct scattering amplitude in the direction K_β. Suppose that we consider the wave function, $\Psi_{K_\alpha^{(1)}}$ corresponding to a plane wave of neutron 1, of unit amplitude, incident along K_α while both neutrons 1 and 2 are scattered[46]. Then the scattering amplitude of neutron 1 along K_β is $f(K_\alpha^{(1)}, K_\beta^{(2)})$. A Green's function satisfying (10.2) is

46. This is in conflict with the exclusion principle but convenient for our present considerations. By superposing the symmetrical wave function, with a negative sign, a solution obeying the exclusion principle can, of course, be obtained.

$$G(r_1, r_1') = \frac{e^{iK|r_1 - r_1'|}}{4\pi |r_1 - r_1'|} + \tag{10.3}$$

$$+ \frac{1}{4\pi f(K_\alpha^{(1)}, K_\beta^{(1)})} e^{i K_\alpha^{(1)} \cdot r_1} \cdot e^{-i K_\beta^{(1)} \cdot r_1'}$$

It satisfies the differential equation and asymptotic conditions of the wave function only where $r_1 \to \infty$, but not where $r_2 \to \infty$, and thus not over the entire asymptotic space (see section II.1., D.1.).

Proceeding nonetheless we write the wave equation (6.5) for our system in the form

$$(\nabla_{r_1}^2 + K^2)\, \Psi_{K_\alpha^{(1)}}(\rho_1, r_1) = - U(\rho_1, r_1)\, \Psi_{K_\alpha^{(1)}}(\rho_1, r_1) \tag{10.4}$$

where

$$-U(\rho_1, r_1) \equiv -\frac{4}{3} \nabla_{\rho_1}^2 + v_{23} + v_{31} + v_{12} - \epsilon_D \tag{10.5}$$

is a kind of effective potential, acting on particle 1 when r_1 is small.

From (10.2), (10.3) and (10.4) we can deduce in the usual way that the wave function satisfies the integral equation

$$\Psi_{K_\alpha^{(1)}}(\rho_1, r_1) = \int G(r_1, r_1')\, U(\rho_1, r_1')\, \Psi_{K_\alpha^{(1)}}(\rho_1, r_1')\, (dr_1'). \tag{10.6}$$

as may also be checked directly. For large r_1 in the direction K_β and small values of ρ_1 this becomes

$$\Psi_{K_\alpha^{(1)}}(\rho_1, r_1) \longrightarrow \frac{1}{4\pi f(K_\alpha^{(1)}, K_\beta^{(1)})}\left(e^{iK_\alpha^{(1)}\cdot r} + f(K_\alpha^{(1)}, K_\beta^{(1)})\frac{e^{iKr_1}}{r_1}\right).$$

(10.7)

$$\int e^{-iK_\beta r_1'} U(\rho_1, r_1') \Psi_{K_\alpha^{(1)}}(\rho_1, r_1')(dr_1').$$

Thus again, regardless of the $\Psi_{K_\alpha^{(1)}}(\rho_1, r_1')$ used in the right hand side of (10.6), the left hand side has the correct scattering amplitude along . However unless splits for large r_1' into a product of the form

$$\Psi_{K_\alpha^{(1)}}(\rho_1, r_1') \longrightarrow \varphi(\rho_1)\, F(r_1') \tag{10.8}$$

$U\Psi_{K_\alpha^{(1)}}$ does not vanish so that (10.6) would diverge. For in contrast to $\lambda f(r)$, U is not a simple multiplicative factor and "cuts off" only wave functions of the type (10.8).

Now consider the expression

$$I = \int \Psi_{-K_\beta^{(1)}}\left(\nabla_{r_1}^2 + K^2 + U(\rho_1, r_1)\right)\Psi_{K_\alpha^{(1)}}(dr_1)(d\rho_1). \tag{10.9}$$

Clearly, for the correct $\Psi_{K_\alpha^{(1)}}$, $I = 0$. Let us now consider the variation of I, if we admit only trial functions of the form

$$\Psi_{K_\alpha^{(1)}} = \int G(r_1, r_1')\, U(\rho_1, r_1')\, \Phi_{K_\alpha^{(1)}}(\rho_1, r_1')(dr_1') \tag{10.10}$$

where $\Phi_{K_\alpha^{(1)}}$ will be suitably restricted; and $\Psi_{-K_\beta^{(1)}}$ is unrestricted. Then

$$\delta I = \int \left\{ \Psi_{-K_\beta^{(1)}}(-D)\,\delta\Psi_{K_\alpha^{(1)}} - \delta\Psi_{K_\alpha^{(1)}}(-D)\,\Psi_{-K_\beta^{(1)}} \right\} (dr_1)(d\rho_1) \tag{10.11}$$

As in section I.6., (6.8) - (6.13) this leads to surface integrals over the five dimensional surfaces $\Sigma_a^{(1)}\ (r_1 = a)$ and $\Sigma_a^{(2)}\ (r_2 = a)$. The one over $\Sigma_a^{(2)}$ vanishes because $\Psi_{K_\alpha^{(1)}}$ has the correct $f(K_\alpha^{(1)}, K_\beta^{(1)})$ owing to its expression in terms of a Green's function. The one over $\Sigma_a^{(2)}$ vanishes if $\delta\Psi_{-K_\alpha^{(1)}}$ describes only outgoing waves of neutron 2, since $\Psi_{-K_\beta^{(1)}}$ contains only such waves and hence the integrand vanishes.

We shall show that $\delta\Psi_{K_\alpha^{(1)}}$ has indeed this property (of outgoing neutron-2 waves) if only $\Phi_{K_\alpha^{(1)}}$ has it. For $r_2 = a$ and $r_1 \leq a$, ρ_1 exceeds 2/3 a.
Hence, by our assumption,

$$\Phi_{K_\alpha^{(1)}} \simeq \varphi(\rho_2) \cdot f\,\frac{e^{iKr_2}}{r_2} \tag{10.12}$$

Now for $\rho_1 \geq$ 2/3 a, (10.12) is an exact solution of the wave equation (10.4) so that

$$\left[\nabla_{r_1}^2 + K^2 + U(r_1\rho_1)\right]\Phi_{K_\alpha^{(1)}} = 0 \tag{10.13}$$

Hence

$$\begin{aligned}
\Psi_{K_\alpha^{(1)}} &= \int G(r_1, r_1')\, U(\rho_1, r_1')\, \Phi_{K_\alpha^{(1)}}(\rho_1, r_1')\, dr_1' \\
&= -\int G(r_1, r_1')\,(\nabla_{r_1}^2 + K^2)\,\Phi_{K_\alpha^{(1)}}(\rho_1, r_1')\,(dr_1') \\
&= -\int \Phi_{K_\alpha^{(1)}}(\rho_1, r_1')\,(\nabla_{r_1}^2 + K^2)\, G(r_1, r_1')\,(dr_1')
\end{aligned} \tag{10.14}$$

(10.14 cont'd)

$$-\int_{r_1'=a} \left\{ G(r_1, r_1') \nabla_{r_1} \bar{\Phi}_{K_\alpha^{(1)}}(\rho_1, r_1') - \bar{\Phi}_{K_\alpha^{(1)}}(\rho_1, r_1') \nabla_{r_1} G(r_1, r_1') \right\} dS.$$

But when $\rho_1 \geq 2/3\ a$, and $r_1' = a$, $\bar{\Phi}_{K_\alpha^{(1)}}(\rho_1, r_1') = 0$, so that the surface integral vanishes. Hence, using (10.2), we find

$$(10.15) \quad r_2 \longrightarrow \infty : \bar{\Psi}_{K_\alpha^{(1)}} = \bar{\Phi}_{K_\alpha^{(1)}} = \varphi(\rho_2) f \cdot \frac{e^{iKr_2}}{r_2}$$

as was to be shown.

Therefore if the trial function $\bar{\Phi}_{K_\alpha^{(1)}}$ satisfies the conditions

$$(10.16) \quad \bar{\Phi}_{K_\alpha^{(1)}} \begin{cases} \nearrow \text{the product form } \varphi(\rho_1) F(r_1), & \text{as } r_1 \to \infty \\ \searrow \varphi(\rho_2) f \cdot \dfrac{e^{iKr_2}}{r_2}, & \text{as } r_2 \to \infty \end{cases}$$

the equation

$$0 = I = \int \bar{\Psi}_{-K_\beta^{(1)}}(\rho_1, r_1)\, U(\rho_1 r_1)\, \bar{\Phi}_{K_\alpha^{(1)}}(\rho_1, r_1)(d\rho_1)(dr_1)$$

$$(10.17) \quad + \int \bar{\Psi}_{-K_\beta^{(1)}}(\rho_1, r_1)\, U(\rho_1, r_1)\, \frac{e^{iK|r_1 - r_1'|}}{4\pi |r_1 - r_1'|} \cdot U(\rho_1, r_1')\, \bar{\Phi}_{K_\alpha^{(1)}}(\rho_1, r_1')(d\rho_1)(dr_1)(dr_1')$$

$$+ \frac{1}{4\pi f(K_\alpha^{(1)}, K_\beta^{(1)})} \int \bar{\Psi}_{-K_\beta^{(1)}}(\rho_1 r_1)\, U(\rho_1 r_1)\, e^{iK_\alpha^{(1)} \cdot r_1} \cdot e^{-iK_\beta^{(1)}}\, U(\rho_1 r_1')\, \bar{\Phi}_{K_\alpha^{(1)}} (d\rho_1)(dr_1)(dr_1').$$

provides a stationary expression for $f(K_\alpha^{(1)}, K_\beta^{(1)})$.

In this way we can obtain the amplitude for elastic scattering in all directions. In the simple case of n - d scattering, the amplitude for exchange scattering is then determined owing to the restrictions to which the scattering matrix is subject. Thus, let us consider a sub - matrix (S_{ij}^L) corresponding to scattering with a given angular momentum, L, where the subscripts refer to the incoming and outgoing neutrons. There are two modes of disintegration so that, by section I.7. (S_{ij}^L) involves at most three arbitrary constants. In fact, due to the equality of the two neutrons this number is further reduced to two. Thus a single diagonal element completely defines the matrix. It is clear therefore that the determination of $f(K_\alpha^{(1)}, K_\beta^{(1)})$, from which all elements S_{11}^L, can be deduced is sufficient.

Variational principles for $f(K_\alpha^{(1)}, K_\beta^{(2)})$ can be obtained in a similar way, but in addition to volume integrals, as occur in (10.17) they also involve surface integrals. The same holds for variational expressions for the proper phases of the scattering matrix.

No numerical application of (10.17) or its equivalent for the phase shifts has been made. The labour involved would be enormous. Thus the calculation for the phase shifts involves a six dimensional integral which can be reduced to five dimensions by an analytical integration. The remaining integral, owing to the presence of the Green's function must be evaluated numerically. Furthermore, since

the iteration (10.10) extends only over three dimensions, it is not certain how much it improves the trial function and hence one cannot be sure that (10.17) will yield very good results.

CONCLUSION.

The problem of many particle nuclear collisions is a difficult one. Even in classical mechanics the treatment of several interacting particles is in general complicated and hence one cannot reasonably expect a royal road to the solution of the corresponding nuclear problems.

As remarked earlier, however, good results have been obtained for many particle bound states, with a reasonable expenditure of effort and time. In Parts I and II we have examined the two methods which have been used for bound systems, for their applicability to collision processes.

We believe that the Rayleigh-Ritz method, discussed in Part I, provides a practical procedure also for the solution of collision problems. To be sure, the fact that the trial functions must satisfy certain asymptotic conditions (e.g. (6.14)) causes some complication. But the integrals to be evaluated in a collision calculation are of precisely the same kind as occur in the binding energy calculation of the corresponding bound state. This indicates that scattering cross sections can be obtained by an amount of numerical work comparable to that involved in bound state calculations.

On the other hand, the variation iteration method (Part II), although yielding strikingly good results in two body collision problems, appears to be unsuited for the treatment of more complicated scattering processes. For we have seen that the theoretically most satisfactory procedure

(section II.2.) is completely useless from a practical point of view, while other methods (section II.3.) are still extremely complicated and of doubtful value. Of course one cannot rule out the possibility that some better iteration procedure exists. However any integral formulation increases the dimensionality of the integrals to be found. Thus, unless some unforeseen simplification can be made, we do not believe that any such method can be as useful as the Rayleigh-Ritz method.

While this paper falls far short from providing a complete solution of the problem of composite nuclear collisions, it is hoped that it has made some contribution towards paving the way for a systematic treatment of such processes.

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K745 Kohn
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nuclei.